Theory Tools for R-matrix Fitting

2nd Consultants' Meeting on R-matrix Codes
IAEA, Vienna

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Topics

Building on results of Consultants' Meeting last December

1. Need to apply standard R-matrix formalism
2. Translation code Ferdinand (ferdinand.py)
3. Other Code Development
4. Comparisons
5. Discussion of fitting p + ^{27}Al resonances
6. Needed future work

Applying standard R-matrix formalism

Sometimes approximations are convenient!

- B=S approximation for shift functions (as in SAMMY)
- Reich-Moore approximation with diagonal damping (see ORNL)
- Using potential scattering for a baseline and adding R-matrix terms for extra resonances (as in SigmaCalc)
- Using Breit-Wigner resonances as baseline (early SigmaCalc)
- Non-relativistic vs relativistic kinematics (see LANL)

Would be ok if these could be translated to standard formalism

- But not all these are are translatable (yet).

Translation code 'Ferdinand'

- Written in Python 2, using Fudge processing for GND.
- Translates to & from: gnd, endf, sfresco, azure, hyrma*

  * in development
- Brune transformations to (and Barker from) Brune's formalism
  - Barker: specify any energy-independent boundary condition B
- New 'PoPs' database being implemented ('Properties of Particles')
  - Add or remove particle-pair channels
  - Change elastic channel
- Will show results for n + ^{16}O, p + ^{27}Al.

ENDF format

Extract for masses, and ½+ spin-parity set

```
   8016.0   1.585751+1          0          0          1          0 825 2151    1
   8016.0   1.000000+0          0          0          1          0 825 2151    2
 1.000000-5 6.120000+6          1          7          0          1 825 2151    3
      0.0                       0          3          9          0 825 2151    4
      0.0        0.0            3          0         36          6 825 2151    5
0.000000000 1.685750+1      0.0        8.0        1.0        0.0   825 2151    6
0.000000000      0.0        0.0      102.0        0.0        0.0   825 2151    7
1.000000000 1.585750+1      0.0        8.0        0.5        0.0   825 2151    8
0.000000000      1.0        0.0        2.0        0.0        1.0   825 2151    9
3.967131320 1.289164+1      2.0        6.0        0.0       -0.5   825 2151   10
-2213760.00      1.0        0.0      800.0        1.0        0.0   825 2151   11
      0.5        0.0             0          0         18          3 825 2151   12
      1.0        0.0        0.0        0.0                         825 2151   13
      2.0        0.0        0.5        0.0   4.150000-1 4.150000-1 825 2151   14
      3.0        1.0       -0.5        0.0   6.683904-1 6.683904-1 825 2151   15
      0.0        0.0             0          4         24          4 825 2151   16
-3477455.99 2.500000-1 3.967946+6                                   825 2151   17
2377270.881 2.500000-1 1.619406+5                                   825 2151   18
4060821.280 2.500000-1 1.114238+5 3.482406+3                        825 2151   19
4467364.094 2.500000-1 1.565648+4 2.116526+3                        825 2151   20
```

GND format in XML

Extract for radii, and ½+ spin-parity set

```
<resolved lowerBound="1e-5 eV" upperBound="6.12e6 eV" formalism="R_Matrix_Limited">
  <R_Matrix_Limited approximation="Reich_Moore" calculatePenetrability="true">
    <channels>
      <channel label="0" name="gamma + O17" ENDF_MT="102">
        <link xlink:href="/reactionSuite/reactions/reaction[@label='51']"/></channel>
      <channel label="1" name="n + O16" ENDF_MT="2">
        <link xlink:href="/reactionSuite/reactions/reaction[@label='0']"/>
        <scatteringRadius>
          <constant value="4.15 fm"/></scatteringRadius></channel>
      <channel label="2" name="He4 + C13" ENDF_MT="800" Q="-2213760 eV">
        <link xlink:href="/reactionSuite/reactions/reaction[@label='47']"/>
        <scatteringRadius>
          <constant value="6.683904 fm"/></scatteringRadius></channel></channels>
  <spinGroup index="0" spin="1/2" parity="+">
    <resonanceParameters>
      <table rows="4" columns="4">
        <columnHeaders>
          <column index="0" name="energy" units="eV"/>
          <column index="1" name="gamma + O17 width" units="eV" L="0" channelSpin="0.0"/>
          <column index="2" name="n + O16 width" units="eV" L="0" channelSpin="0.5"/>
          <column index="3" name="He4 + C13 width" units="eV" L="1" channelSpin="-0.5"/></columnHeaders>
        <data>
         <!--     energy | gamma + O17 |  n + O16 | He4 + C13  -->
         <!--            |      width  |   width  |    width   -->
              -3477455.99          0.25    3967946           0
              2377270.881          0.25   161940.6           0
               4060821.28          0.25   111423.8    3482.406
              4467364.094          0.25   15656.48    2116.526</data></table></resonanceParameters></spinGroup>
```

ferdinand.py - main options

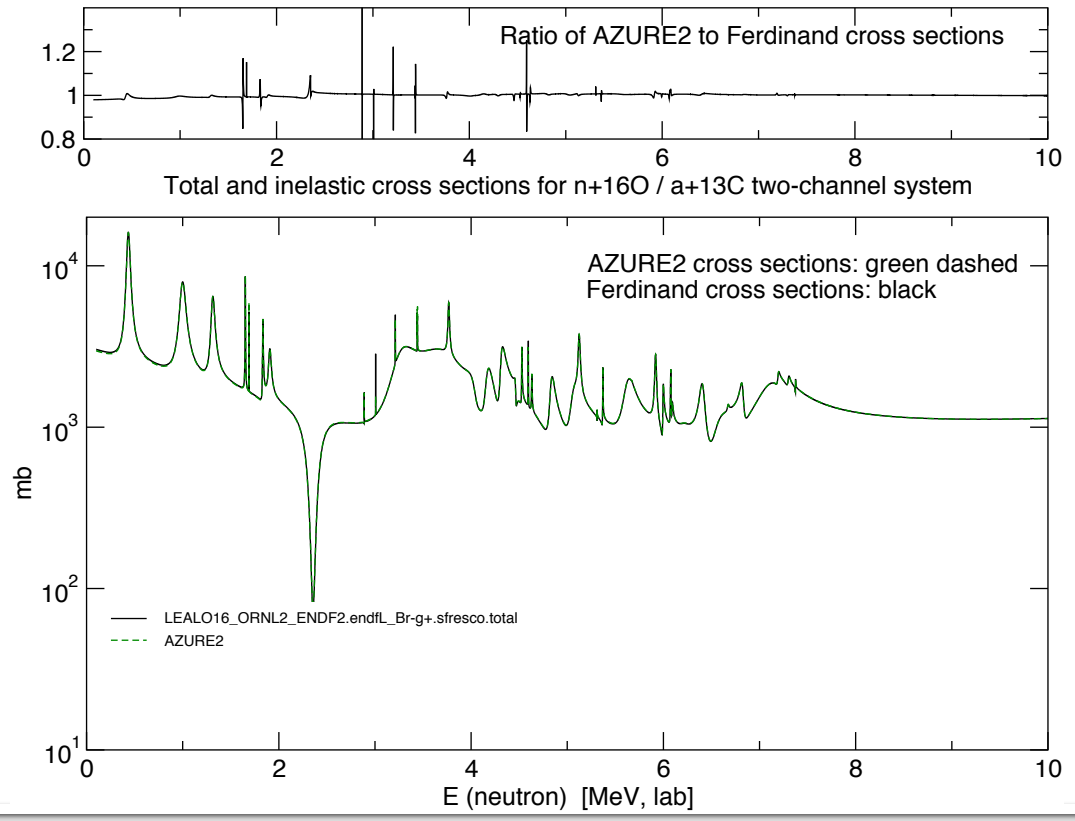
```
usage: ferdinand.py [-h] [-i INITIAL] [-o OUTPUT] [-z] [-v] [-g] [-R] [-r]
                    [-f FILTER] [-e ELASTIC] [-l LOWER] [-u UPPER] [-a] [-G]
                    [-b BOUNDARY] [-t TRANSFORM] [-c] [-E ENERGY] [-F FILE]
                    inFile finalformat

Translate R-matrix Evaluations

positional arguments:
  inFile                The input file you want to translate.
  finalformat           Output source format: fresco, sfresco, hyrma, endf,
                        azure, gnd=xml, ..

optional arguments:
  -h, --help            show this help message and exit
  -z, --zero            Omit zero widths
  -g, --nogamma         Omit gamma channels
  -R, --ReichMoore      Add a Reich-Moore gamma channel and convert to KRM=3
  -r, --noreac          Omit all nonelastic (reaction) channels
  -e ELASTIC, --elastic ELASTIC
                        Index (1,2,..) of elastic particle-pair
  -f FILTER, --filter FILTER
                        Filter of csv list of particle-pairs to include, e.g.
                        1,3,4 (no blanks). Overrides -g,-r options
  -a, --amplitudes      Convert intermediate gnd file stores to reduced width
                        amplitudes, not widths.
  -G, --Gammas          Convert intermediate gnd file stores to formal widths,
                        not reduced width amplitudes. Overrides -a.
  -b BOUNDARY, --boundary BOUNDARY
                        Boundary conditions for output file for EDA or FRESCO:
                        'C,X' where C=L,B,k,E or S, and X=float for B,k and E
  -t TRANSFORM, --transform TRANSFORM
                        Transform 'Brune' or 'Barker' of pole specification
```

Other Code Developments

- Need pointwise-reconstruction of cross sections from the R-matrix parameters (energies, widths, channels, B values)
  - Use numerical form for Rutherford cross section (not integrable)
- Reconstruction of charged-particle elastic cross section
  - RECENT in PREPRO: not yet implemented
  - SAMMY: implemented
  - Fudge: being implemented by Caleb Mattoon and Dave Brown
  - in principle, any R-matrix fitting code can output the needed data
- Need implementation of Brune parametrization
  - SHF=2 in ENDF6 format. Nov 2017: ask CSEWG; fix pointwise translation
  - GND option agreed. May 2017: ask SG-38 (et al) at WPEC
  - Already available in Ferdinand, Hyrma, ..

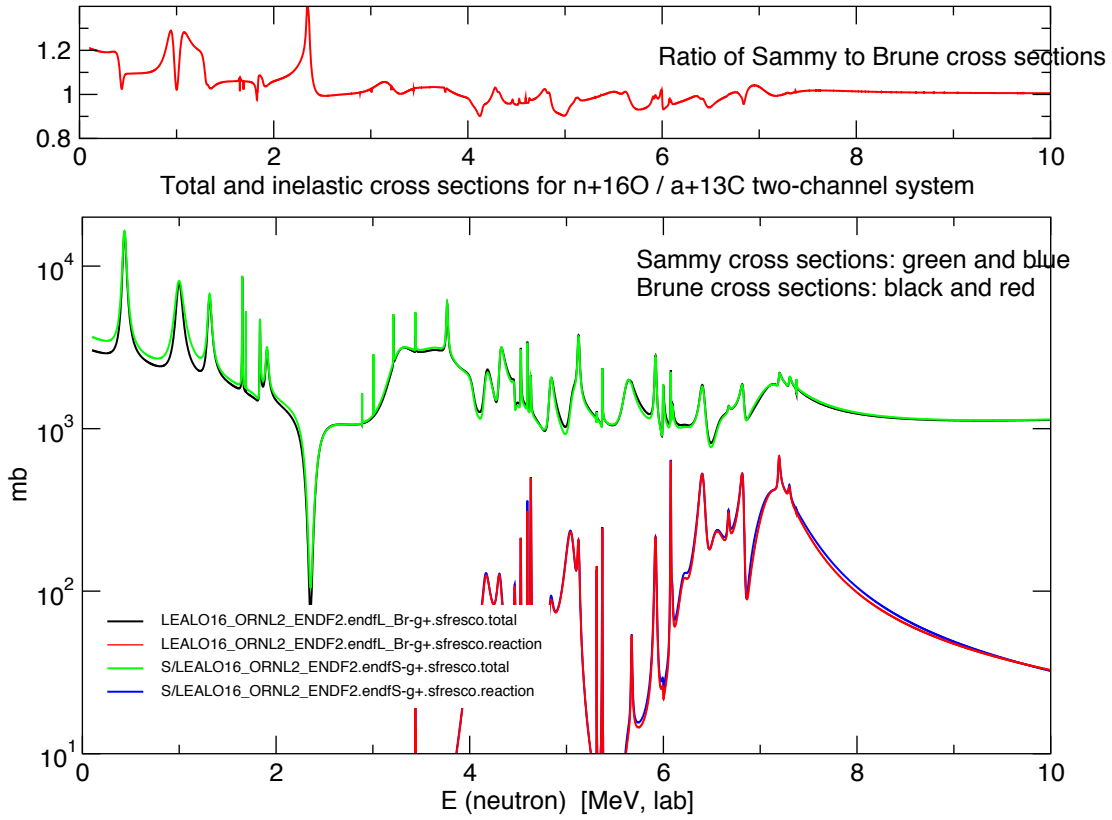
Comparisons for n + ^{16}O (1)

- For reference, use parameter fits from Luiz Leal for 0 to 6 MeV
  - Although this used the S=B approximation of SAMMY
  - So pretend these numbers are Brune transform, then translate back.
- Then:
  SFRESCO agrees well with AZURE2.



Comparisons for n + ^{16}O (2)

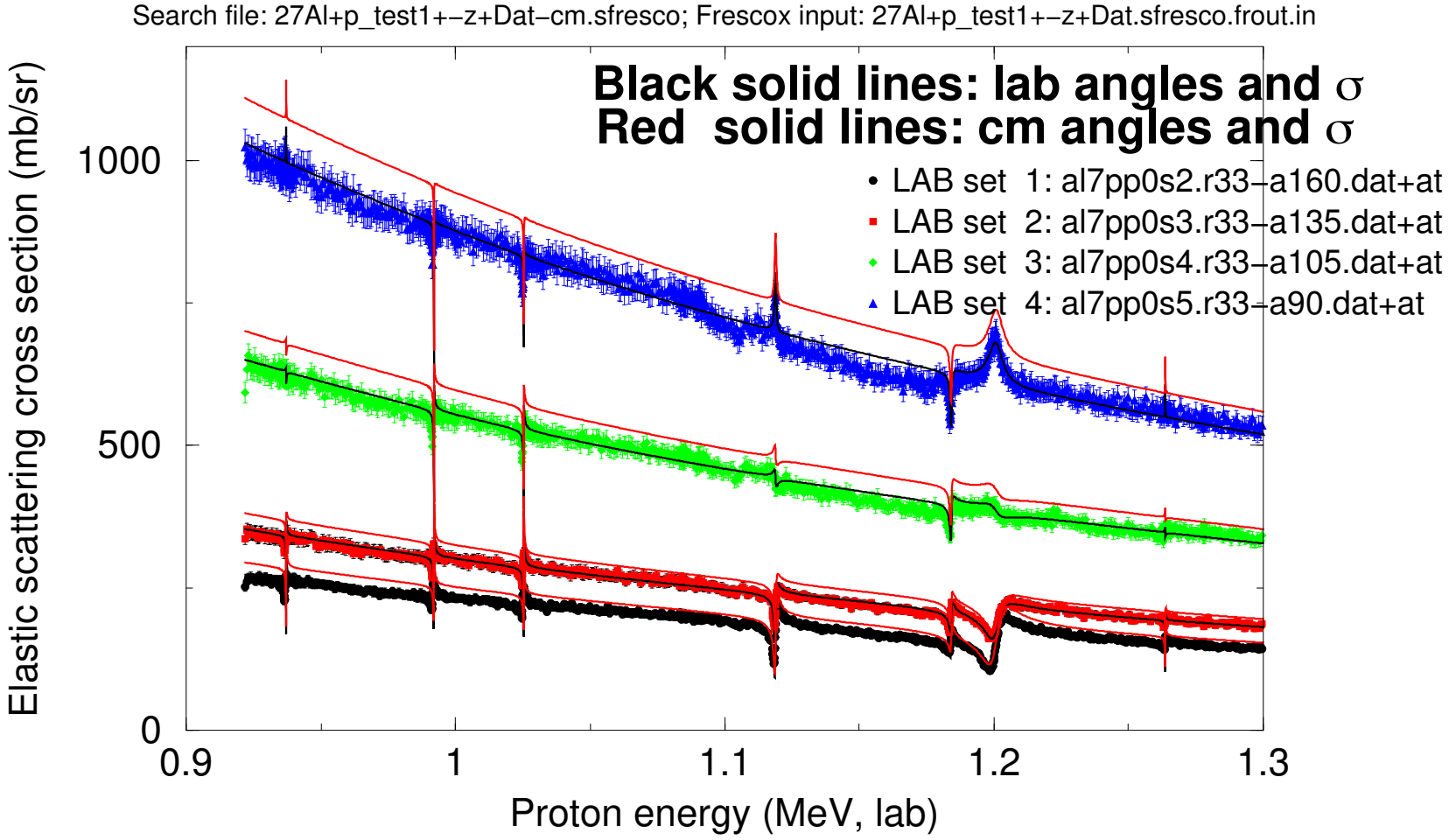
- For reference, use parameter fits from Luiz Leal for 0 to 6 MeV
  - Although this used the S=B approximation of SAMMY
- What is affect of S=B approximation?
- See different cross sections between resonances.



Fitting p + ^{27}Al resonances

- Clarifying the experimental data from EXFOR database
  - Lab or cm angles? Lab or cm cross sections?
  - Proton energy calibration?
- Nelson(thesis, 1983, p50): "At lower energies, where the off-resonance cross sections were predominantly Rutherford, the data were normalized to the fit by the sums of the areas under the calculated and experimental excitation functions"
- I find:
  Only by treating EXFOR data as for lab angles and lab cross-sections do I approach Rutherford at low energies.

Treating Nelson data as lab or cm?



Global χ^2/N reduces from 27.6 to 16.8

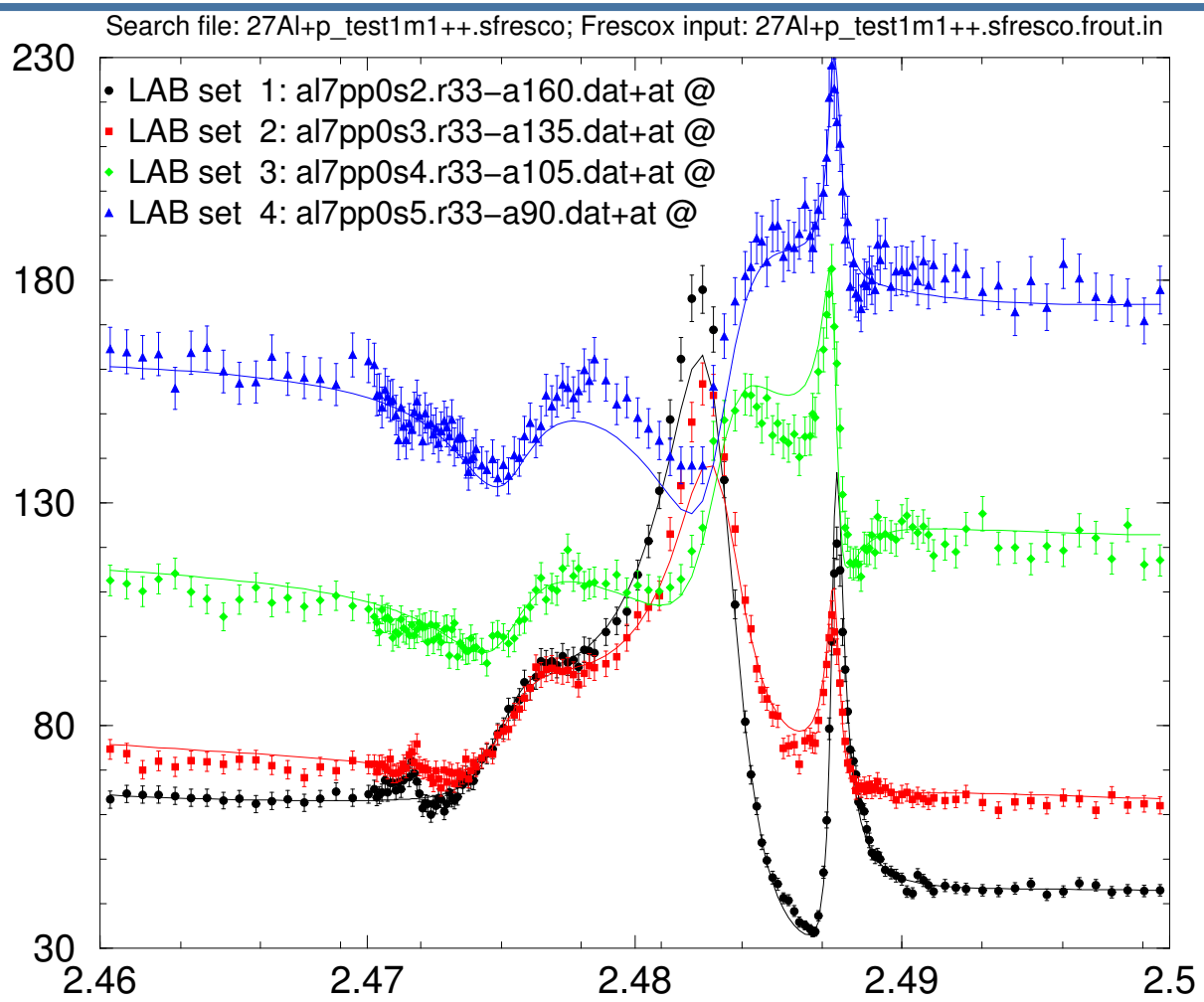
Calibration of Proton energies

- Nelson (PRC 29, 1984): "Absolute energy calibrations were based on the resonances in ^{27}Al(p,g) at Ep = 991.90±0.04 keV (Ref 10, Roush) and 1799.75±0.09 kev (Ref 11, Maas)"
- I find lower resonance 2.4 keV too low, upper resonance 3.2 keV too high !
  And a resonance at 2814 keV too high by 10.9 keV.
- Paper does talk of "uncorrected laboratory energies".
- I recommend rescaling the experimental energies (MeV) by
  E(new) = E(old) – (9.75 – 7.308*E(old))/1000
- Global χ^2/N reduces from 40.4 to 16.14 for 4 scattering angles

My strategies for fitting

- Use existing tables of energies, spins and parities wherever possible! At least as starting points for iterations
- Very convenient to start as if Brune (or even B=S) energies
- I do not have a good strategy for searching for E/J/π values from scratch. Or, to make widths of new channels.
- I find it useful to focus on a specific resonance (or group) by
  (a) keeping all R-matrix parameters in calculation
  (b) but vary only those parameters near the resonance, and
  (c) calculate and plot only energies near resonance.

Example of regional fit of p + ^{27}Al resonances



Elastic resonances in region of 2.45 – 2.50 MeV.

Four scattering angles.

Future developments needed

- Release ferdinand.py
  - when fudge is stable, and released. Hope: Jan 2017
- Implement and check pointwise-reconstruction for all processing that needs charge-particle elastic scattering
  - Fudge
  - replacement for PREPRO?
- Dealing with data: scaling, broadening, correlations, discrepant,
- Covariances
  - Extract parameter covariance matrix from final chi-squared fit,
  - Write these to evaluations (e.g. MF=32 in ENDF6 format)
  - Check with users of evaluated R-matrix covariances!
- DO WHOLE EVALUATIONS, merging R-matrix and HF results.

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