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RSPt

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RSPT IN THEORY

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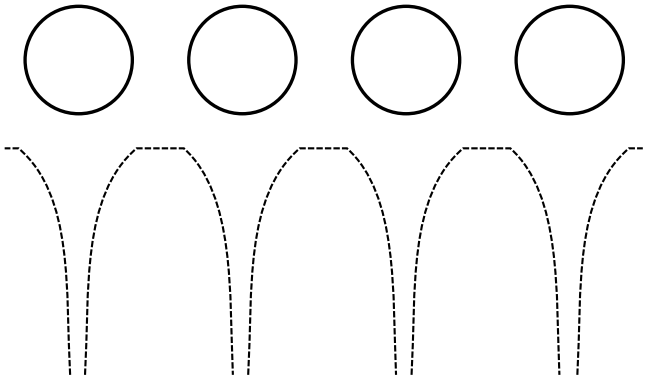
What is RSPt?

RSPt

- Relativistic Spin-Polarized toolkit
- a tool to calculate the properties of a system of many interacting electrons
  - standard density functional theory (LDA/GGA)
    - ✓ for non- or weakly-correlated electron systems
  - dynamical mean-field theory
    - ✓ weakly-correlated electron systems
    - ✓ strongly correlated electron systems

The basis

- full-potential linear muffin-tin orbital method (FP-LMTO)



$$\psi_{lm}^{MTO}(\varepsilon,\kappa,\mathbf{r}) = \mathcal{Y}_{lm}(\hat{\mathbf{r}}) \begin{cases} \phi_l(\varepsilon,r) + \mathcal{J}_l(\kappa,r)\cot\left[\eta_l(\varepsilon)\right] & \texttt{MT} \\ \mathcal{K}_l(\kappa,r) & \texttt{INT} \end{cases}$$

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RSPt features

- full-potential LMTO with spin-polarization
- all electron code
- scalar relativistic with spin-orbit coupling
- fully parallelized over k-points and atoms
- SIC, LDA+U, and LDA+DMFT implementations
- inter-atomic magnetic exchange parameters

Features close to completion:

- fully relativistic implementation
- non-collinear magnetism
- XAS

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What can RSPt do for us?

- equilibrium volumes of materials
- cohesive energies
- valence configuration
- elastic constants
- magnetic moments
- one-particle excitation spectra
- band structures
- Fermi surfaces
- dielectric tensor and XMCD spectra

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When to use RSPt?

- fully relativistic → accurate even for open structures
- when accurate total energies are needed
  - magneto-crystalline anisotropy (MAE)
  - relative phase stability (crystallographic, magnetic)
  - when studying a wide range of pressures
- for compounds consisting of rare-earth or actinide elements
- for strongly correlated materials:
  - iron chalcogenides (LaFePO, …)
  - non-magnetic oxides (VO_2, …)
  - Fe_3O_4
  - manganites
  - transition metal elements: Ni
  - nuclear fuel materials (UO_2, …)

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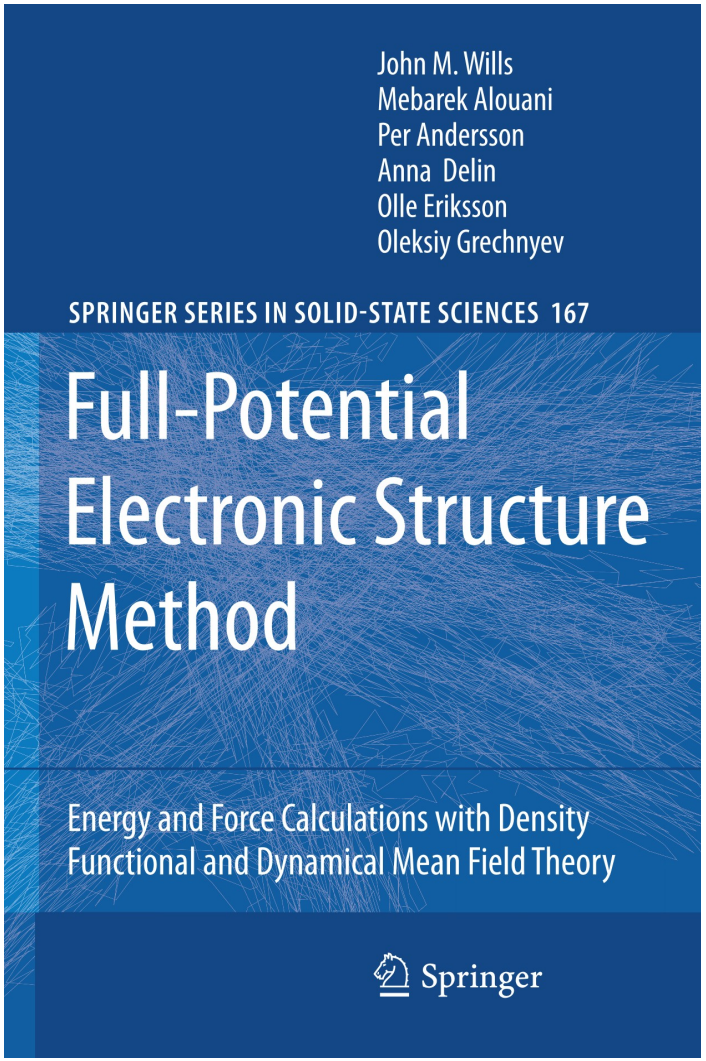
The reference book



http://www.springer.com/cn/book/9783642151439

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RSPT IN PRACTICE

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How to get started?

- `symt.inp`
  - defines the geometry
  - chemical species at different sites
  - what kind of calculations one wants to perform

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Example of a symt.inp file

```
# Lattice constant in a.u.:
lengthscale
10.8691376094
# Lattice vectors (columns)
latticevectors
  1.000000000000000   0.000000000000000  -0.504820026296751
  0.000000000000000   0.788949354104004   0.000000000000000
  0.000000000000000   0.000000000000000   0.787970573866038
# Spin axis
spinaxis
  0.000000000000000   0.000000000000000   0.000000000000000  l
# Sites
atoms
12
  0.239470000000000   0.978940000000000   0.026460000000000   23 l 4e_V    # V
  0.760530000000000   0.021060000000000   0.973540000000000   23 l 4e_V    # V
  0.760530000000000   0.478940000000000   0.473540000000000   23 l 4e_V    # V
  0.239470000000000   0.521060000000000   0.526460000000000   23 l 4e_V    # V
  0.106160000000000   0.211850000000000   0.208590000000000    8 l 4e_01   # O1
  0.893840000000000   0.788150000000000   0.791410000000000    8 l 4e_01   # O1
  0.893840000000000   0.711850000000000   0.291410000000000    8 l 4e_01   # O1
  0.106160000000000   0.288150000000000   0.708590000000000    8 l 4e_01   # O1
  0.400510000000000   0.702580000000000   0.298840000000000    8 l 4e_02   # O2
  0.599490000000000   0.297420000000000   0.701160000000000    8 l 4e_02   # O2
  0.599490000000000   0.202580000000000   0.201160000000000    8 l 4e_02   # O2
  0.400510000000000   0.797420000000000   0.798840000000000    8 l 4e_02   # O2
# Perform a spin polarized calculation
#spinpol
# Perform a fully relativistic calculation
#fullrel
```

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Files needed for DFT calculations

- `symcof`
  - defines the symmetry of the lattice
- `atomdens`
  - initial atomic density
- `data`
  - details of the calculation:
    - exchange-correlation functional
    - basis
    - type of mixing, …
- `spts, tetra`
  - defines the sampling of the Brillouin zone

For DMFT: green.inp

```
convergency
1d-6 1d-4 900 300

inputoutput
T T T

spectrum
Hyb Dos Proj

energymesh
4001 -2.0 2.0 0.010

debug
Symmsolver Renorm_corr Dbgout     ! dbgstr

verbose
Sigma Projection Solver Dc Dump   ! verbstr

projection
2

mixing
1  0.10000 0.100

! Ni 3d type 1
cluster
1 2 eV                            ! ntot udef [nsites] [e_unit]
1 2 1 1 0 6.00 0.95               ! t l e site basis, U J or F0 F2 F4 (F6)
6 2 0.3                           ! solv DC sigma_mix [symbrk]
8 0 -4 2.0 6 10                   ! ed_nelec, ed_nextra, ed_nenvextra, ed_n, ed_nfit, ed_sweight
0.000 0.0
```

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Now run(s)…

```
#!/bin/bash -l
# The -l above is required to get the full environment with modules

# Set the allocation to be charged for this job
# not required if you have set a default allocation
#SBATCH -A 2017-00-00

#SBATCH --mail-user my.email@physics.uu.se
#SBATCH --mail-type=ALL

# The name of the script is myjob
#SBATCH -J myjob

#SBATCH -t 24:00:00

# Number of nodes
#SBATCH -N 8
#SBATCH --ntasks-per-node=32
# Number of MPI processes.
#SBATCH -n 256

#SBATCH -e error_file.e
#SBATCH -o output_file.o

module swap PrgEnv-cray PrgEnv-intel
module swap intel/14.0.4.211 intel/15.0.1.133
module unload cray-libsci

/../rspt-1.1/bin-sandibridge/runs "aprun -n 256 /../rspt-1.0/bin-haswell/rspt" 1e-13 100
```

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Technical details

- written in Fortran and C
- makes use of BLAS, LAPACK, and FFTW → Intel MKL
- MPI parallelism over k-points, and atoms
- available for GPU as well
- ~~NPAR, NSIM, KPAR~~
- "-DMEMORY_STORE"

  → keep more in memory, write less to file

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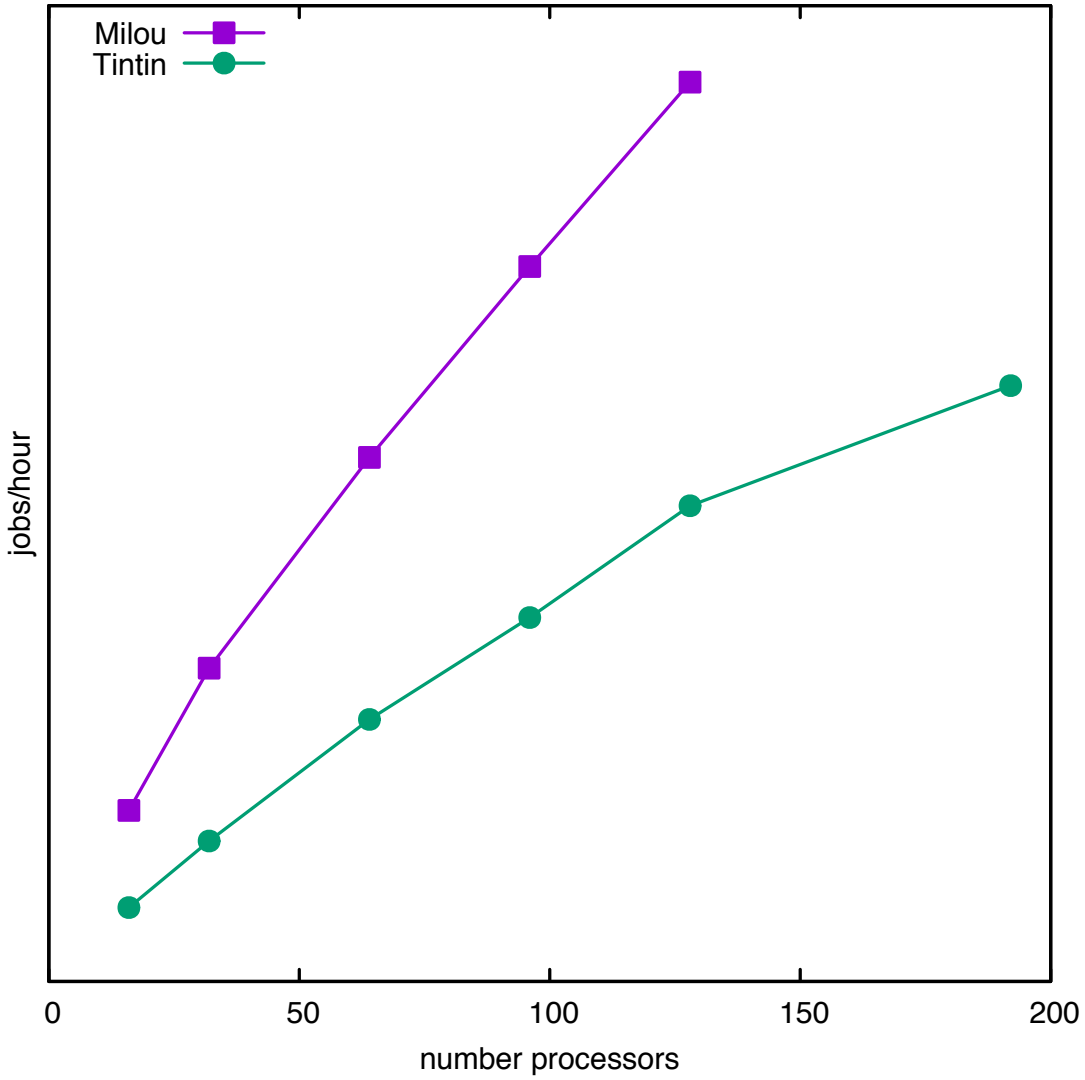
Scaling @UPPMAX



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How many nodes or processors should I use?

- RSPt is parallelized over k-points

  ➟ very good scaling (~linear) up to

  number of processors = # of k-points

  ✓ for relatively small cells

- RSPt is also parallelized over atoms and bands

  number of processors = # of k-points x *i*

  i = 2, 3, …, 8

Keep yourself updated about RSPt!

- in constant development in order to introduce new features and optimizations
- the RSPt webpage:
  - http://fplmto-rspt.org
  - forum
  - latest release of the code
  - RSPt schools and workshops
- for developers
  - GitHub
  - UU, KTH, Los Alamos National Lab, Strasbourg Univ.
- email me: at diana.iusan@physics.uu.se