CSSI Element: A General and Effective B-Spline R-Matrix Package for Charged-Particle and Photon Collisions with Atoms, Ions, and Molecules

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Introduction

- BSR is a general program package to calculate high-quality atomic data for:
  - structure (energy levels, oscillator strengths)
  - photoionization (bound –> free transitions)
  - electron scattering from atoms and ions
- BSR can be run in non-relativistic (LS), semi-relativistic (Breit-Pauli), and full-relativistic (Dirac-Coulomb) mode.
- Data from BSR are used in:
  - fundamental research to support many experiments
  - data-intensive modelling applications, especially in plasma and astrophysics

Goals

- Further development of the code (efficiency; parallelization; more physics: molecules and short-pulse, intense laser-atom interactions)
- Simplification of input and output to facilitate use by non-experts
- Creation of many sample inputs, run scripts, and extensive documentation
- Creation of a website with possibility for questions and feedback
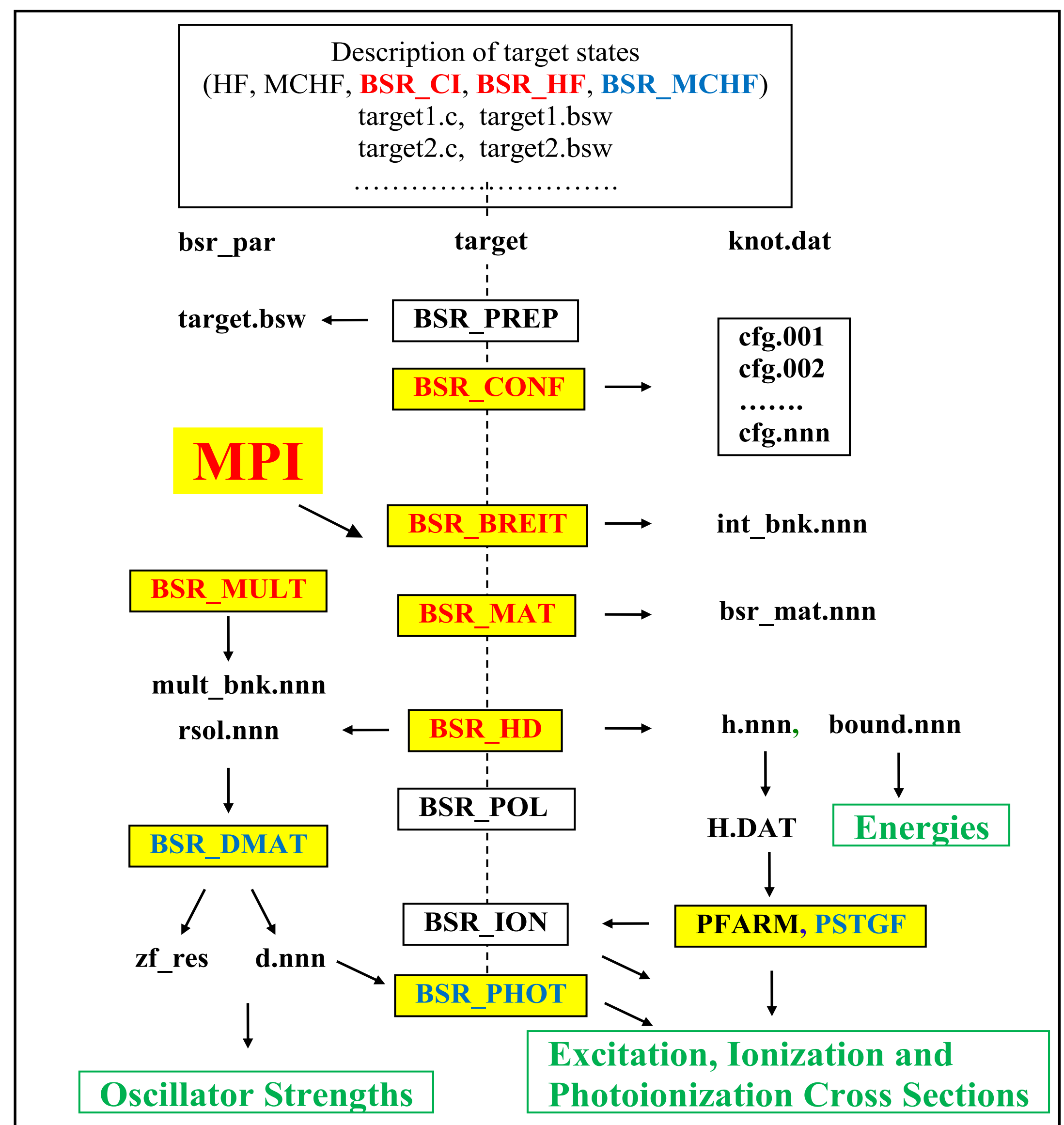- Wide and free distribution via CPC, github, AMP Gateway, etc.

B-spline atomic R-Matrix code (BSR)

```
e + Ca+

coupling = LS    ! coupling scheme
nz     = 20      ! nuclear charge
nelc   = 19      ! number of electrons

ntarg   =  6     ! number of target states

4s              targ_001    0  2  1   -676.59058592  10  9
4d              targ_002    2  2  1   -676.53378783   6  6
4p              targ_003    1  2  -1  -676.47473702  15  6
5s              targ_004    0  2  1   -676.35162078  10  0
3d              targ_005    2  2  1   -676.33047471   6  0
5p              targ_006    1  2  -1  -676.31379441  15  0

nct    =  62     ! total number of target configurations
nwt    =  25     ! total number of target orbitals
nsub   =  11     ! number of substitution orbitals

nlsp   =  14     ! number of partial waves

     8 ==>  order  of splines (ks)
   140 ==>  number of splines (ns)
 20.00000 ==>  nuclear charge (z)
  0.25000 ==>  step size from 0 to 1 (h for z*r, = (1/2)^n)
  0.70000 ==>  maximum step size (hmax for r)
 80.00000 ==>  maximum r (rmax)
```
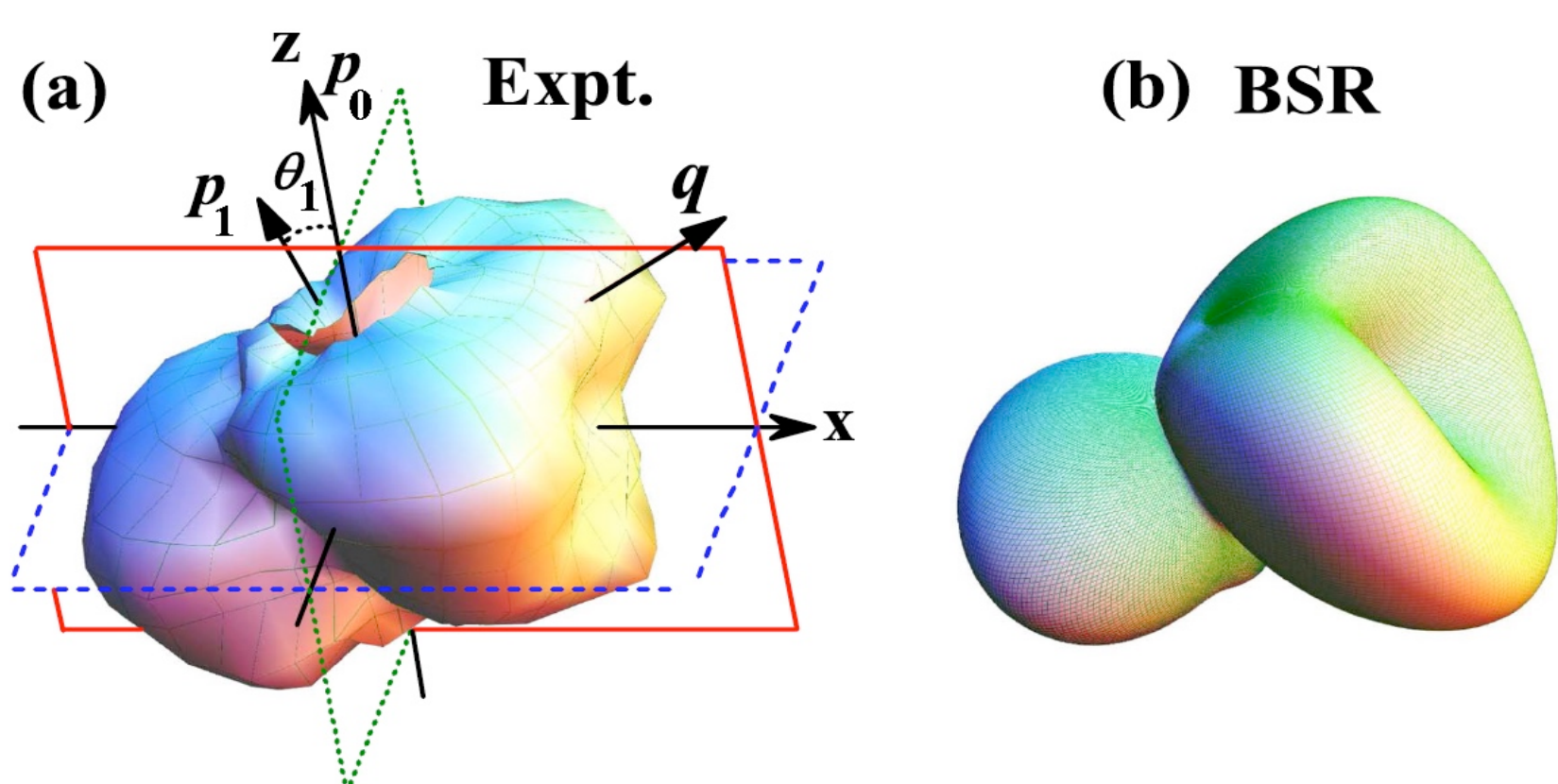
C_bound ▸
C_JK ▸
C_LS ▸
C_phot ▸
Ca_bound ▸
Ca_sct ▸
Fe_photoionization ▸

c 3d.c
3d.w
c 4d.c
4d.w
c 4p.c
4p.w
c 4s.c
4s.w
c 5p.c
5p.w
c 5s.c
5s.w
bsr_par
knot.dat
target

Preview of BSR test suite including sample target and knot.dat files.

- 30,000-50,000 lines of FORTRAN 95 code organized in 10 modules
- Choice between serial and MPI parallelized versions of modules
- (SCA)LAPACK for diagonalization of large matrices
- Human-readable, descriptive BSR input files
- Target-state descriptions can be generated by widely-available non-BSR codes (HF, MCHF, DARC) with plans to include other packages (CIV3, FAC)
- Suite of utilities for processing BSR outputs
- Test suite with sample inputs, outputs, and run scripts for 7 different problems (more to come)
- Fully relativistic (Dirac-Coulomb) DBSR code with similar anatomy is undergoing development

Description of target states
(HF, MCHF, BSR_CI, BSR_HF, BSR_MCHF)
target1.c, target1.bsw
target2.c, target2.bsw
....

bsr_par — target — knot.dat

target.bsw ← BSR_PREP

BSR_CONF → cfg.001 / cfg.002 / ...... / cfg.nnn

MPI

BSR_BREIT → int_bnk.nnn

BSR_MULT — BSR_MAT → bsr_mat.nnn

mult_bnk.nnn

rsol.nnn ← BSR_HD → h.nnn, bound.nnn

BSR_POL — H.DAT — Energies

BSR_DMAT — BSR_ION ← PFARM, PSTGF

zf_res — d.nnn — BSR_PHOT

Oscillator Strengths — Excitation, Ionization and Photoionization Cross Sections

Scientific Impact

(a) Expt. (b) BSR

Fully-differential cross section for **(e,2e) on Ar(3p)**; Ren *et al.*, Phys. Rev. A **93** (2016) 062704; no other theory comes even close to the data.

BSR, $3d^6 4s^2$ a^5D

BSR, $3d^7 4s$ a^5F
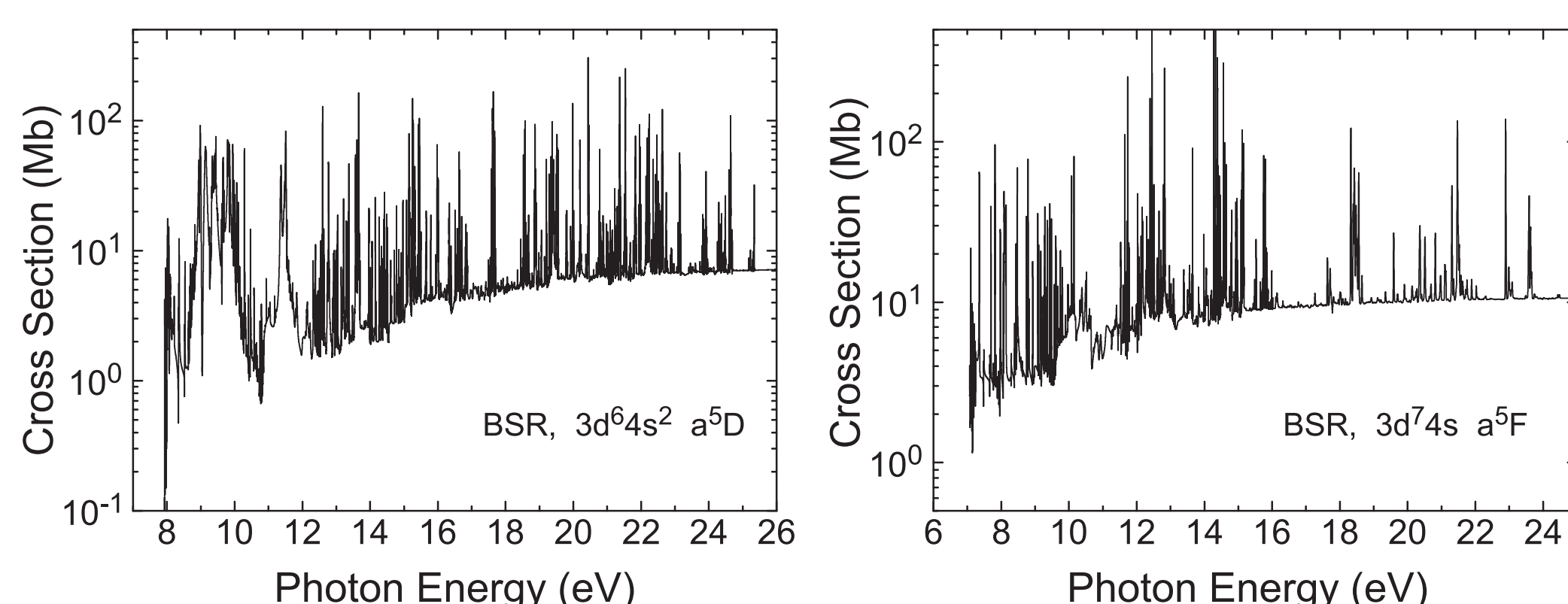
Photoionization of iron from ground and excited states; Zatsarinny *et al.*, Phys. Rev. A **99** (2019) 023430; very complex resonance structure.
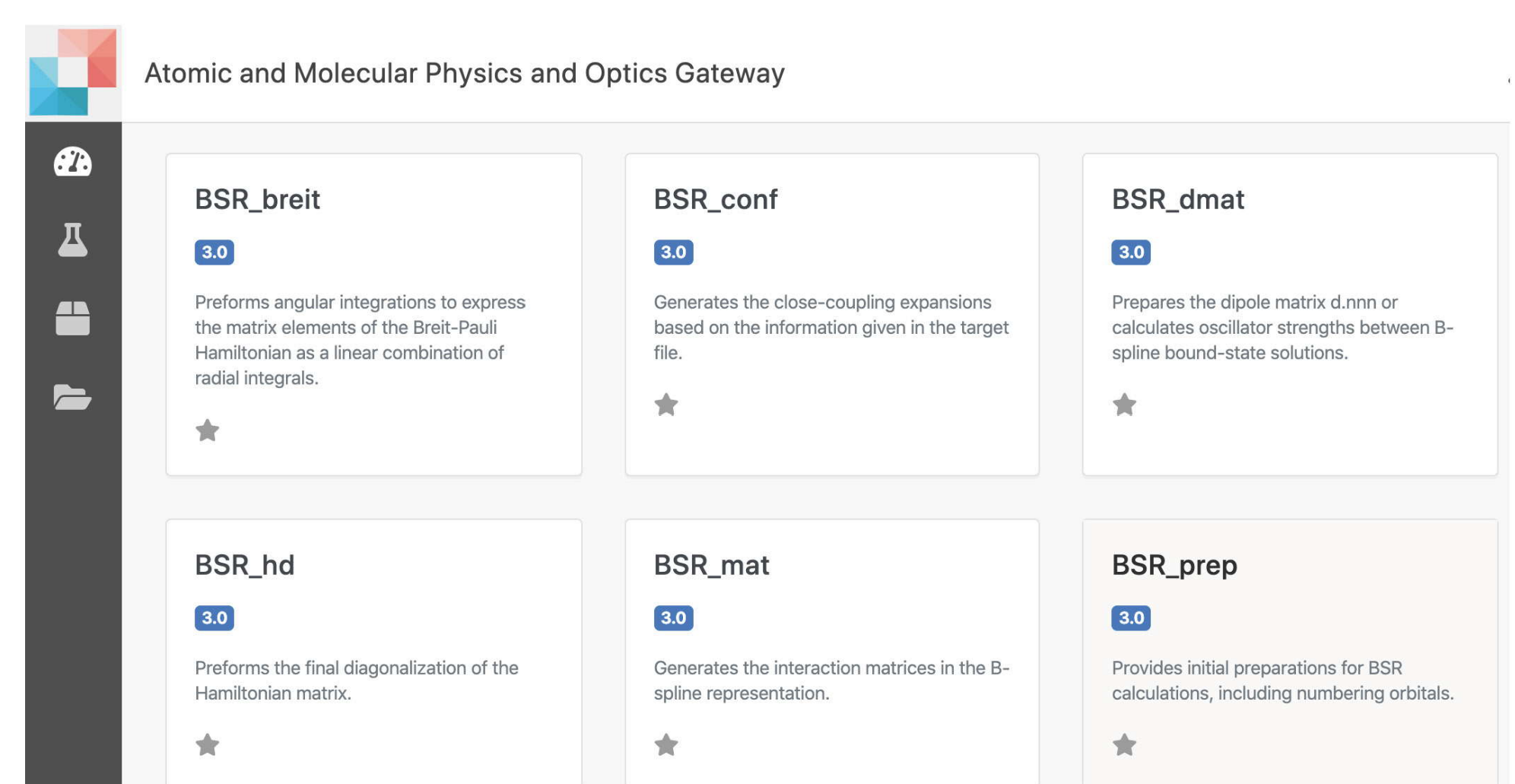
Community Interaction

- first release of BSR downloadable from Computer Physics Communications
- BSR 3.0 available on the AMP Gateway:
  - Gateway is based on Apache Airavata
  - Institutional and individual (sign-up) logins allow access to BSR for researchers and students.
  - Access to XSEDE resources
  - Code documentation hosted on gateway
- Integration with existing open-source time-dependent R-matrix code is currently under development.

BSR CPC

AMP Gateway

Atomic and Molecular Physics and Optics Gateway

BSR_breit 3.0
Preforms angular integrations to express the matrix elements of the Breit-Pauli Hamiltonian as a linear combination of radial integrals.

BSR_conf 3.0
Generates the close-coupling expansions based on the information given in the target file.

BSR_dmat 3.0
Prepares the dipole matrix d.nnn or calculates oscillator strengths between B-spline bound-state solutions.

BSR_hd 3.0
Preforms the final diagonalization of the Hamiltonian matrix.

BSR_mat 3.0
Generates the interaction matrices in the B-spline representation.

BSR_prep 3.0
Provides initial preparations for BSR calculations, including numbering orbitals.

Dashboard of the AMP Gateway.