FISPACT-II & Libraries simulation package

FISPACT-II & Libraries package

1. The directory **/doc** containing user documentation. The report CCFE-R(11)11; the **FISPACT-II User Manual** and all 11 V&V and handbook reports

2. The directory /**fispact** containing the FISPACT-II software. Its directory structure is as follows:

   1. **/exec** - directory containing prebuilt executable (g95, gfortran, ifort, pgfortran, oracle)
      - **Linux** - directory containing Linux executable **(12)**
      - **Mac-OSX** - directory containing Mac OS X executable **(2)**
      - **Windows** - directory containing Windows executable **(2)**

   2. **/source** - software source directory
      - **build** - directory for building an executable using make
      - **build_win** - directory for building an executable using a windows batch file
      - **config** - directory for configuration files
      - **f77** - directory for Fortran 77 source
      - **f90** - directory for Fortran 95 source **62,017 lines of code**

FISPACT-II & library package

3. The software test data directories: ~700 test cases

/getting_started - Tutorial examples described in the User Manual

/fispQA - Validation tests for FISPACT-II using ENDF formatted nuclear data

/fispQA2010 - Validation tests for FISPACT-II using EAF formatted nuclear data and old style input files (not in the next release)

4. The nuclear data directories:

/ENDFdata - TENDL-2014, ENDF/B-VII.1, JENDL-4.0u, JEFF-3.2 libraries and an ENDF version of EAF 2010 data (36 Gb)

+ TENDL-2015 and CENDL-3.1 @ http://www.ccfe.ac.uk/EASY-data/FISPACT-II/

/EAF2010data - EAF 2010 library data (not in the next release)

Total ~40 Gb (6.4 Gb compressed, fits on DL DVD)

FISPACT-II

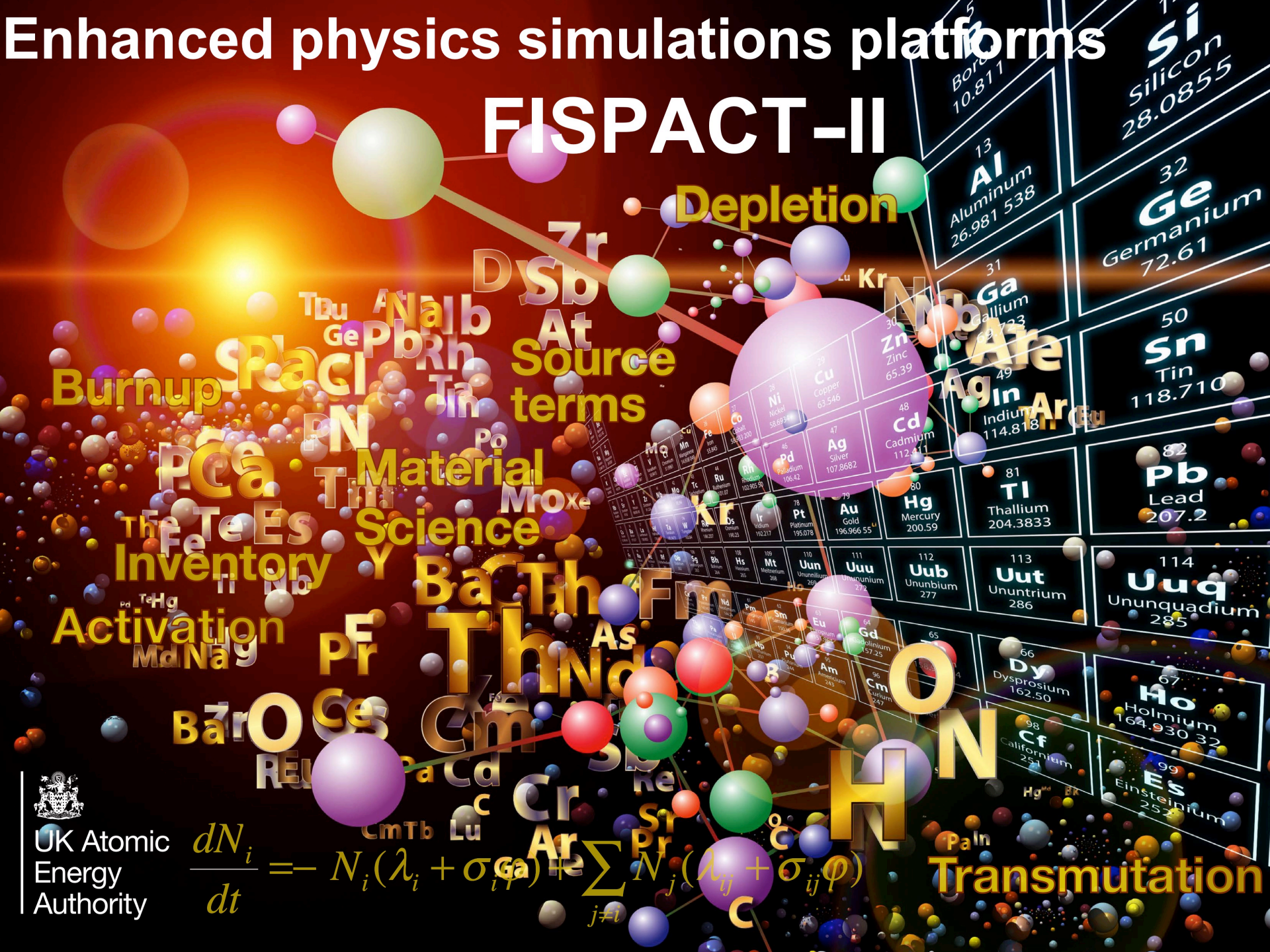
21st century multi-particle inventory code package for stockpile, fuel cycle stewardship, source terms, materials characterization and life cycle management for:

- Magnetic and inertial confinement fusion
- Fission Gen II, III+, IV plants
- Advanced energy and fuel systems
- High energy and accelerator physics
- Medical applications, isotope production
- Earth exploration, Astrophysics
- Homeland security
- …

http://www.ccfe.ac.uk/fispact.aspx

Enhanced physics simulations platforms

FISPACT-II



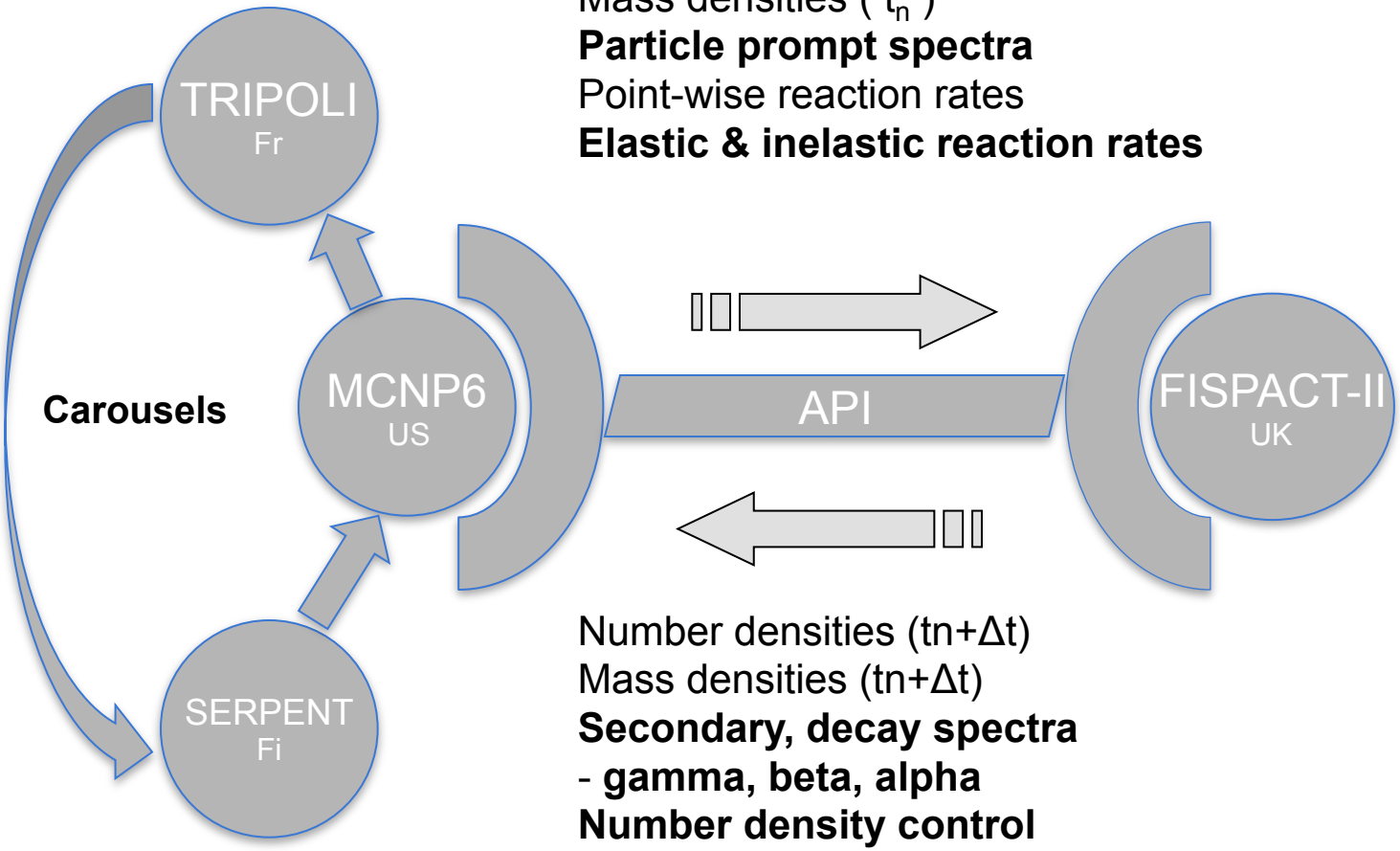
UK Atomic Energy Authority

Simulation in space, energy and time

Boltzmann equation

Number densities (t_n)
Mass densities (t_n)
Particle prompt spectra
Point-wise reaction rates
Elastic & inelastic reaction rates

Bateman equation
(t-dependence of inventories)



ORIGEN US
CINDER US
DARWIN Fr
ACAB SP
ACT4 JA

Number densities (tn+Δt)
Mass densities (tn+Δt)
Secondary, decay spectra
- **gamma, beta, alpha**
Number density control
- **removal, homogenisation, virtual cells, irradiation conditions**

FISPACT-II & Libraries Roadmap

- Enhanced physics
  - Unified Monte-Carlo sampling distributions
  - Charged particle induced ✓ and spontaneous fissions ✓
  - Residual and emitted particle spectra for material science ✓
  - Monte Carlo using covariance input data
  - High energy deep spallation, fission, evaporation (TALYS)
- Coding improvements
  - Multi projectile irradiation ✓
  - Fast library loading ✓
  - Multi-threading, parallelism ✓
- Extended data libraries set: ENDF/B-VII.1, JENDL-4.0u, JEFF-3.2 , CENDL-3.1 ✓
- Automated Verification and Validation processes
- Nuclear data visualisation tools ✓

FISPACT-II & Libraries Roadmap

- Resolve the remaining format-processing issues
- Comprehend, propagate all variance-covariance UQP
- Process the emitted spectra: recoils + p and a
- Wrap up the automated V&V processes; Fusion, Fission, Accelerator V&V
- Update the decay data (tags, g-lines, half-life,…)
- p, d, a and g transmutations
- MACS, 5-30-80 Kev Doppler broaden data files
- More physical information for material's science
- API Application Programming Interface
  - TENDL-2016, TMC's
    - more robust actinides
      - impeccable stables
        - high energy

FISPACT-II 3.10 enhancements

- New graph capabilities
  - beta and gamma block
  - individual nuclide contributions for each observable
- FILE content, info in the input deck, not anymore in the file file
- UQP on targets, parents isotopes
- Materials sciences
  - SPECTRA-PKA and pka libraries
  - Displacement per atom formula Ed as user choice
- JENDL-2015/DDF, JENDL-a and JENDL-FPY-2011

FISPACT-II 3.10 enhancements

- Extend grpconvert capabilities
  - Per unit lethargy, per unit energy in a given energy range
- 1102 groups structures as standard for xs and PT's
- Group structure as free input; read from the xs library directory
- More emitted spectra/particle delayed information
- Better diagnostics
- …

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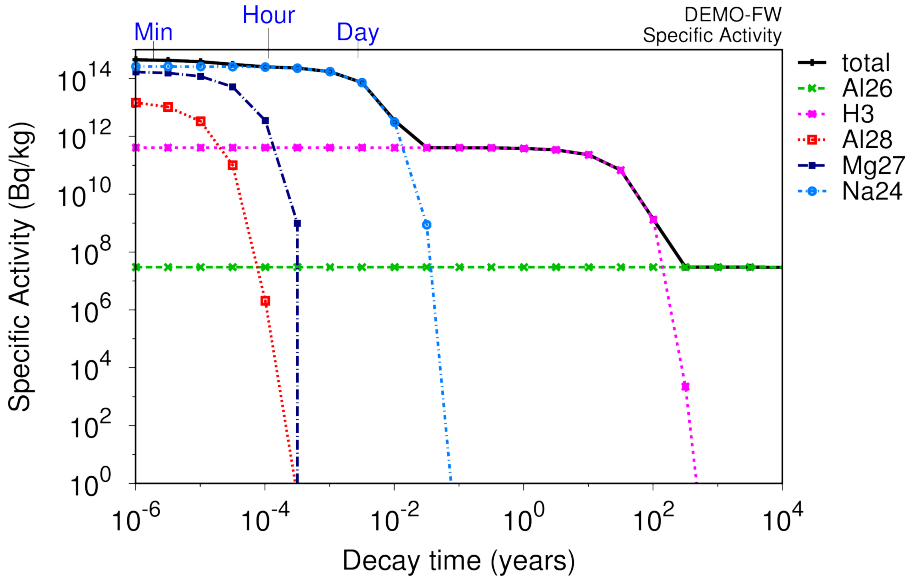
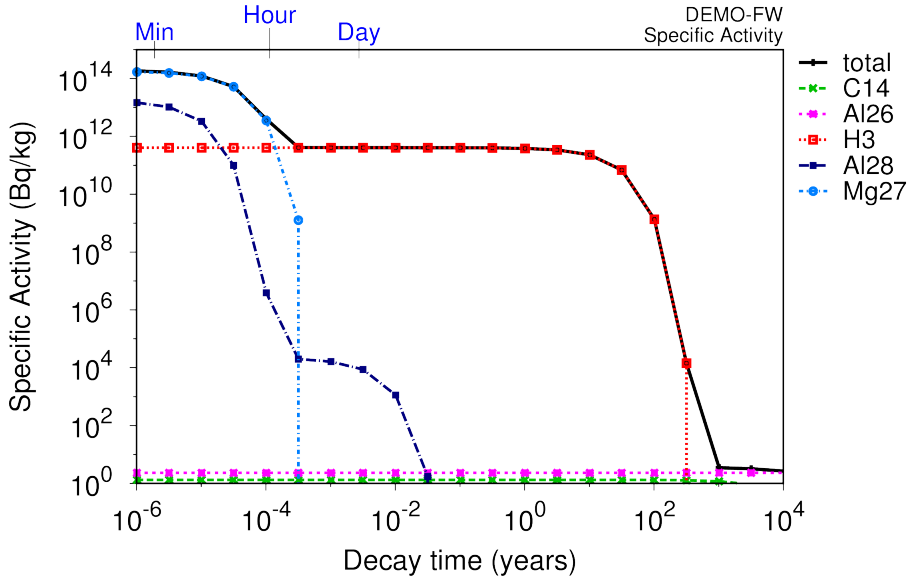
Individual nuclide contributions

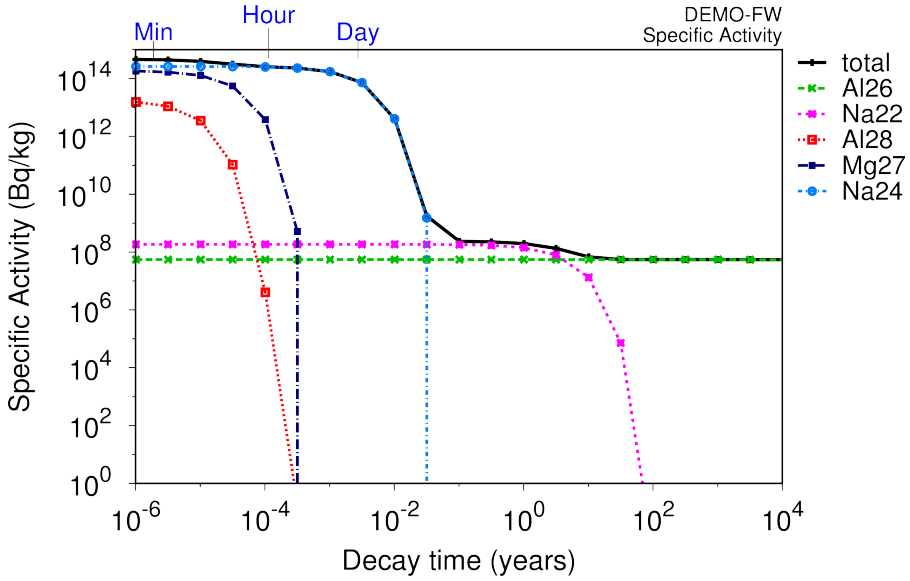
ENDF/B-VII



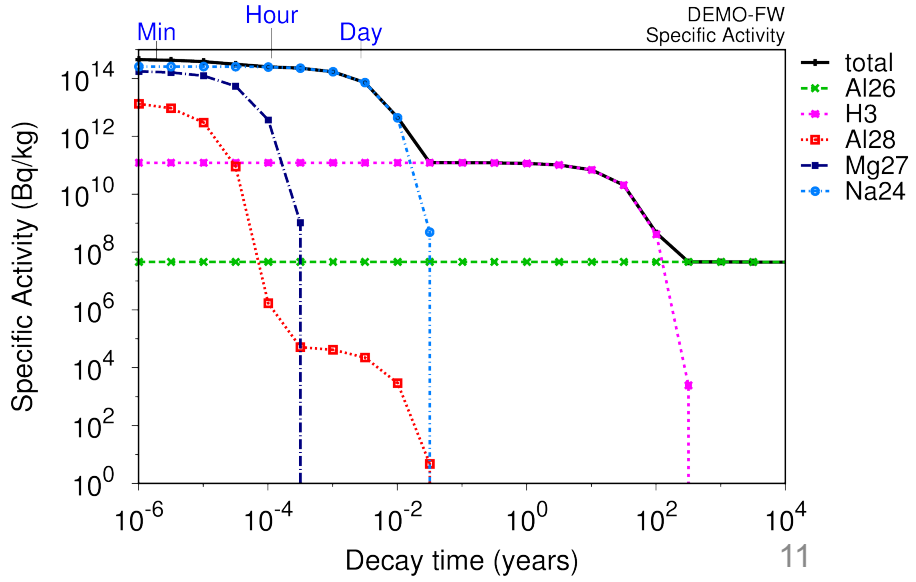
JEFF-3.2



JENDL-4.0



TENDL-2014



FISPACT-II & Libraries

The new and advanced features of FISPACT-II, with enhanced nuclear data forms, provide robust, predictive simulation capabilities, which can be applied to any nuclear system: past, present or future ones

- Web site: http://www.ccfe.ac.uk/fispact.aspx
- Forum e-mail : forum@fispact.ccfe.ac.uk
- Admin e-mail : admin@fispact.ccfe.ac.uk
- Distribution though the OECD/NEA Databank and RSICC at Oak Ridge, educational license only

FISPACT-II distribution policy

Site specific, multi-user licences

FISPACT-II Items	Licence	
	Commercial	Research
• Executable + all data sets • One year's maintenance and minor upgrades	£30k	£15k
• Annual maintenance and minor upgrades	£4.5k	£2.5k
• Source code	Price on demand	
• Training		

Notes

1. Research licences only for academic or public sector research establishments
2. Research licences at a nominal 1£ fee for UK universities, close collaborators and medical applications
3. Research usage does not include contracts