Computational Atomic and Molecular Physics for Transport Modeling of Fusion Plasmas

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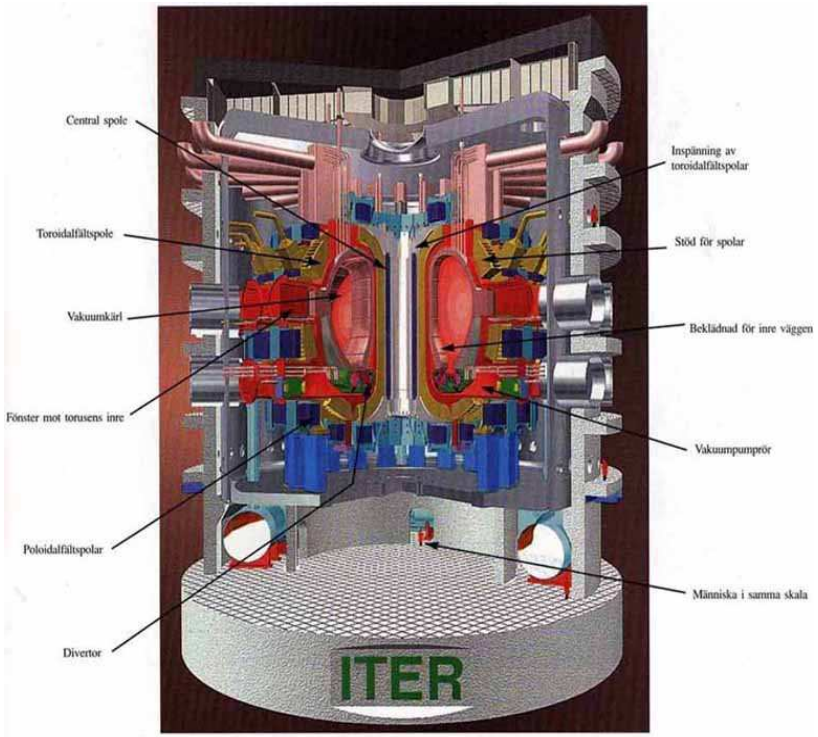
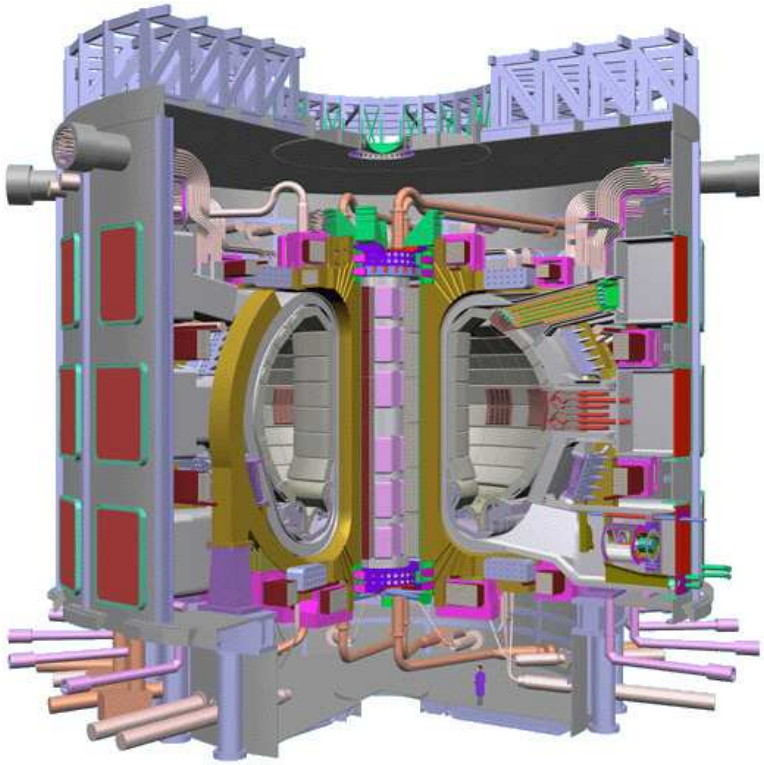
ITER relevance and motivation



- Final choices for plasma-facing materials.
- Relevance of innovations in operational regimes.
- Be, C, and W components for the first wall.
- Study of Edge Localized Mode (ELM) transient in standard ITER operation

ØChief experimental spectroscopic tools and models need reliable atomic data, challenging the state-of-the-art computational methods

ITER relevance and motivation



ØEnhancing the atom data – modeling/diagnostics interface through use of the Atomic Data and Analysis Structure (ADAS)

•Two-dimensional, time dependent, multi-species transport code such as SOLPS (B2-Eirene) uses the ADAS database.

•Used for analysis at JET, ASDEX-Upgrade, DIII-D, JT-60, Tore-Supra, and Alcator C-Mod.

ADAS availability

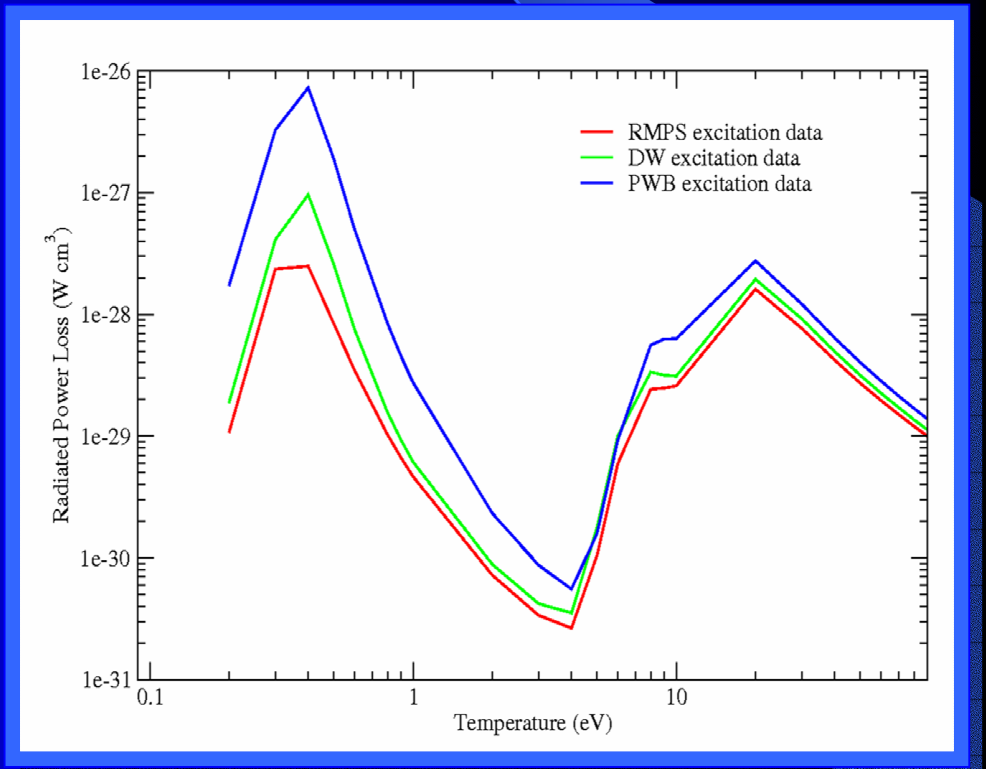
- ADAS is accessible through members of the international consortium such as the ORNL Controlled Fusion Atomic Data Center (CFADC) and General Atomics

- ADAS formatted data generated by this SciDAC project is also directly disseminated via the CFADC website www-cfadc.phy.ornl.gov

Collisional-radiative modeling using ADAS

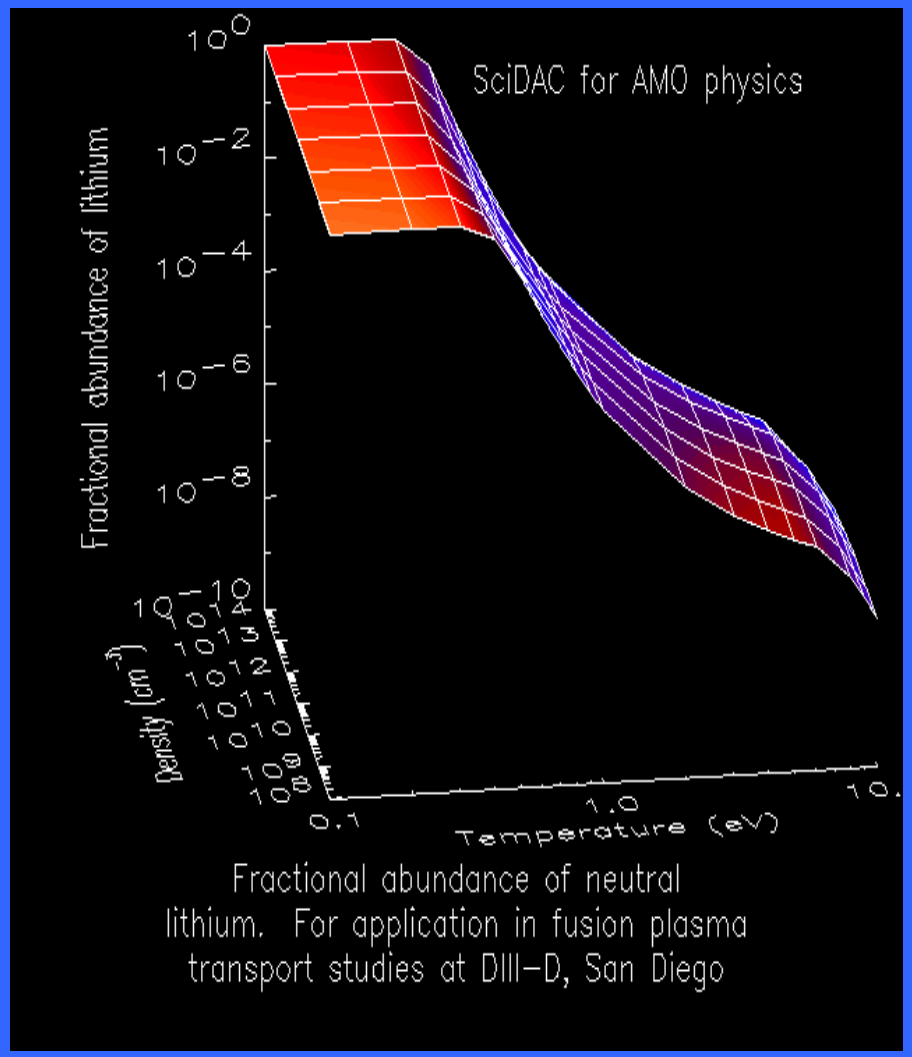
- Developed originally at JET, now used broadly within the fusion and astrophysics communities

- Solution to collisional-radiative equations for all atomic levels in all ionization stages of relevant elements, requiring, e.g.,
  - –Atomic structure for energies
  - –Radiative rates
  - –Collisional electron excitation rates
  - –Collisional electron ionization
  - –Collisional electron recombination rates
  - –Collisional charge transfer recombination



Collisional-radiative modeling using ADAS

- The problem is simplified through the assumption of quasi-static equilibrium for the excited states.
- The following data is produced, for ease of use in plasma transport codes
  - Generalised collisional-radiative (GCR) coefficients
  - Radiated power loss (RPL) coefficients
  - Individual spectrum line emission coefficients
- We have completed the following sequences
  - He, Li and Be



Fractional abundance of neutral lithium. For application in fusion plasma transport studies at DIII-D, San Diego

Electron collision data calculations : Time independent R-Matrix

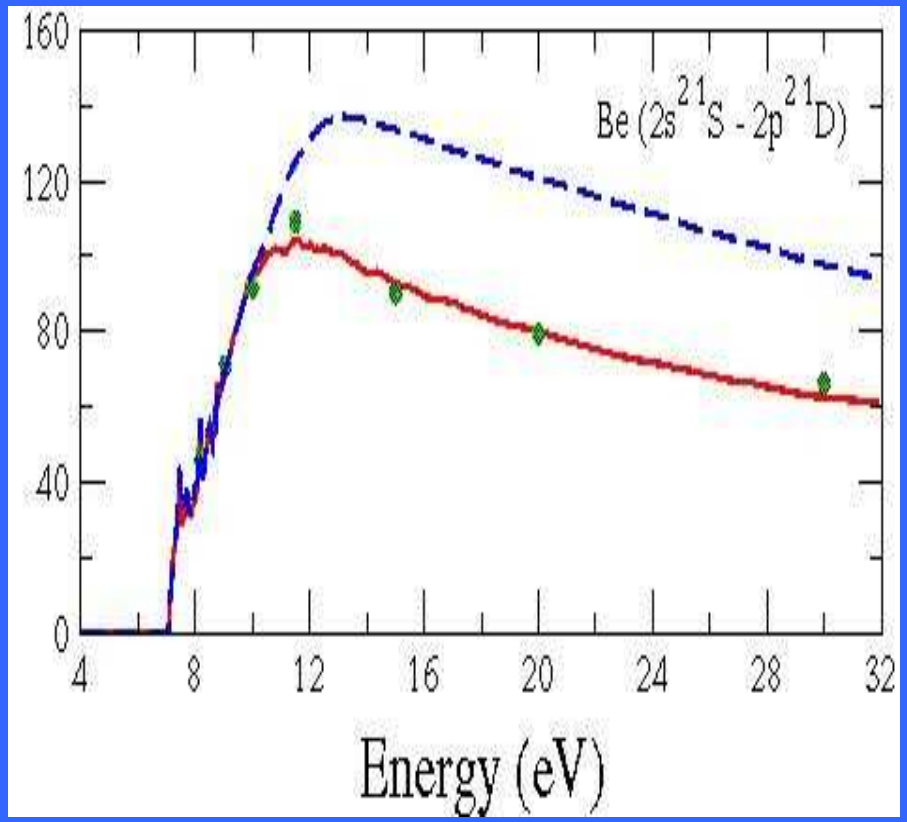
- Originally developed by P.G. Burke and co-workers
- Each atom or ion modeled as an N-electron Hamiltonian
- Collision system modeled as an N+1 electron Hamiltonian
  - Hamiltonian represented by bound and continuum basis states

- All eigenvalues and eigenvectors of 50,000 x 50,000 matrix requiring massively parallel machines
- Thousands of energies required to map out Feshbach resonances also requiring parallel implementations

- Highest priority focus of this SciDAC project – parallel code development and urgent fusion applications

Electron collision data calculations : Time independent R-Matrix

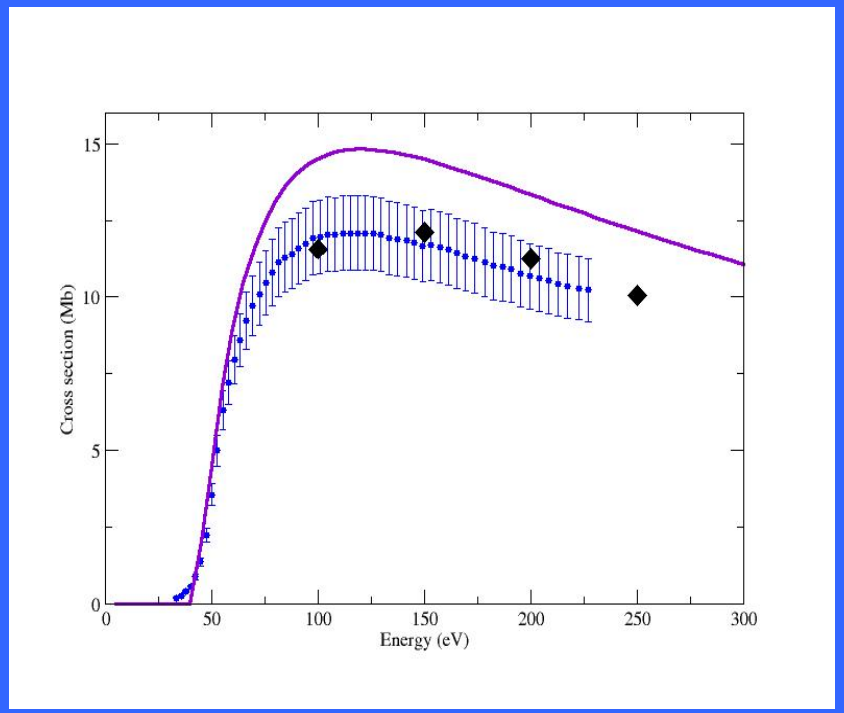
- MPP R-Matrix with pseudo states (RMPS) calculations completed for
  - He, He^{+}
  - Li, Li^{+}, Li^{2+}
  - Be, Be^{+}, Be^{2+}, Be^{3+}
  - B^{+}, B^{4+}
  - C^{2+}, C^{3+}, C^{5+}
  - O^{5+}
- MPP R-Matrix completed for
  - Ne^{+}, Ne^{4+}, Ne^{5+}
  - Fe^{20+}, Fe^{21+}, Fe^{23+}, Fe^{24+}, Fe^{25+}



Energy vs excitation cross section for neutral Be

Electron collision data calculations : Time Dependent Close-Coupling

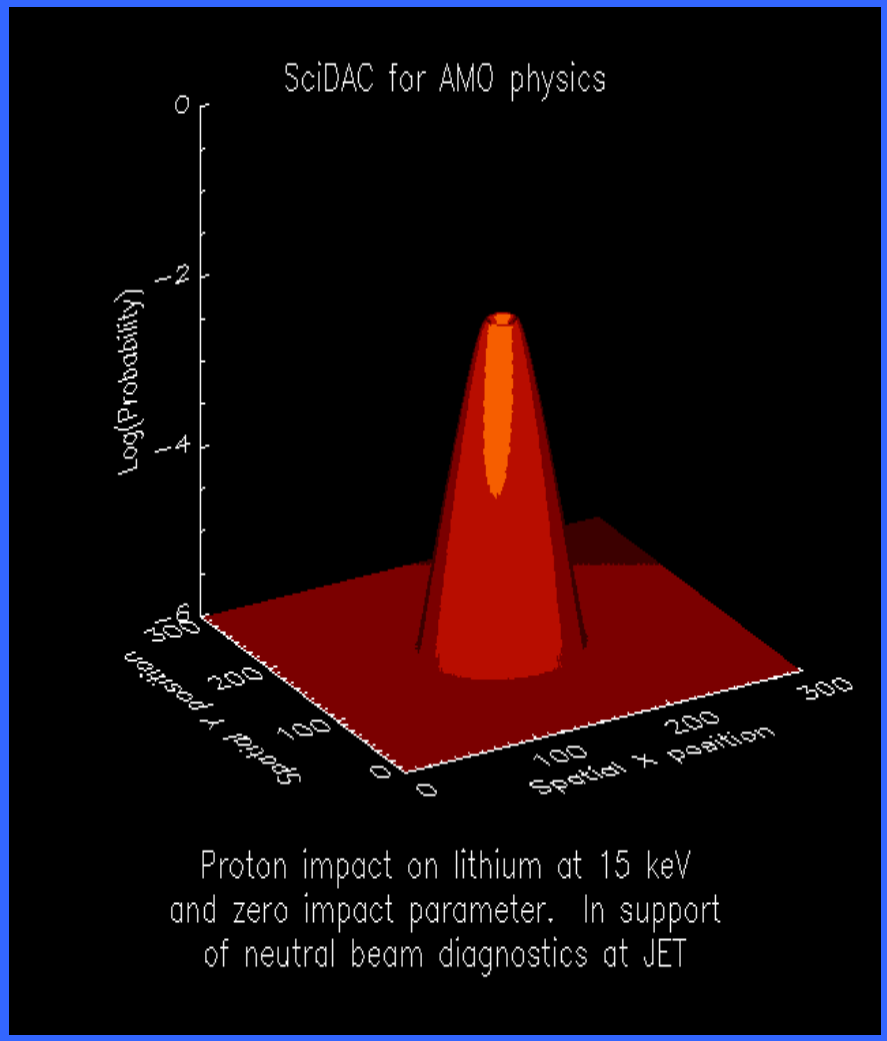
- Pioneered by C. Bottcher and co-workers and developed through SciDAC project, enabled by computational advances
- Treats the three body Coulomb breakup explicitly
- Close-coupled set of 2D lattice equations
- TDCC calculations completed for
  - H, He, He^{+}
  - Li, Li^{+}, Li^{2+}
  - Be, Be^{+}, Be^{2+}, Be^{3+}
  - B^{2+}, C^{3+}, Mg^{+}, Al^{2+}, Si^{3+}



Ionization cross section for C^{2+}. Shows the first agreement between theory and experiment for a system with significant metastable fraction.

Heavy-particle collision data : Lattice, Time-Dependent Schrödinger Equation

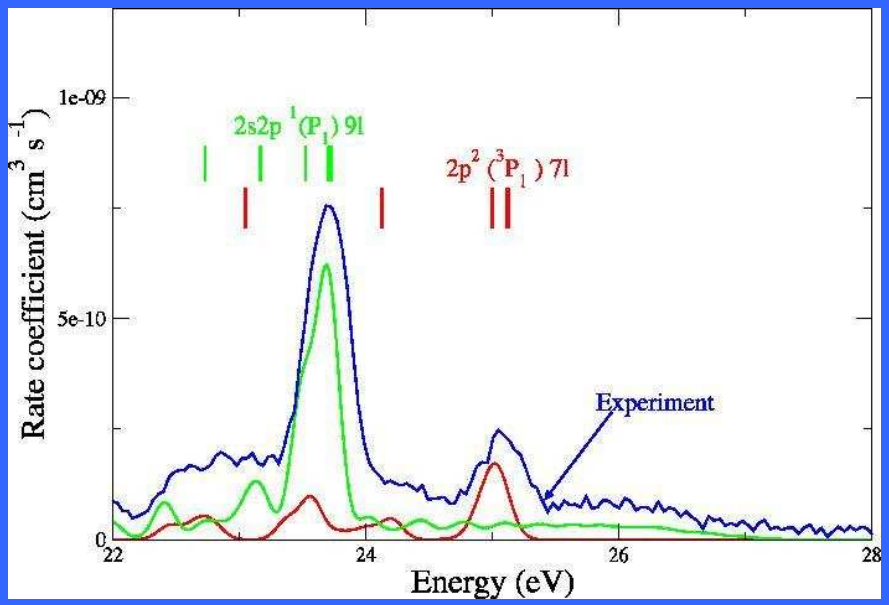
- Electron in the field of two moving Coulomb or model potential fields
- 3D lattice Schrödinger equation solved by low-order finite differences or high-order Fourier-collocation representation, developed by SciDAC team and enabled by computational advances
- Applications
  - p+H, p+Li, α+H, Be^{4+}+H, p+H_2^+
- Hybrid LTDSE/AOCC method



Other methods “unleashed” by advanced computation and computers : Distorted-wave Born approximation and Classical Trajectory Monte Carlo techniques

- DW and CTMC needed for accurate, large-scale electron collision data and radiative and autoionization rates, especially for complex ions such as those of W, Mo.

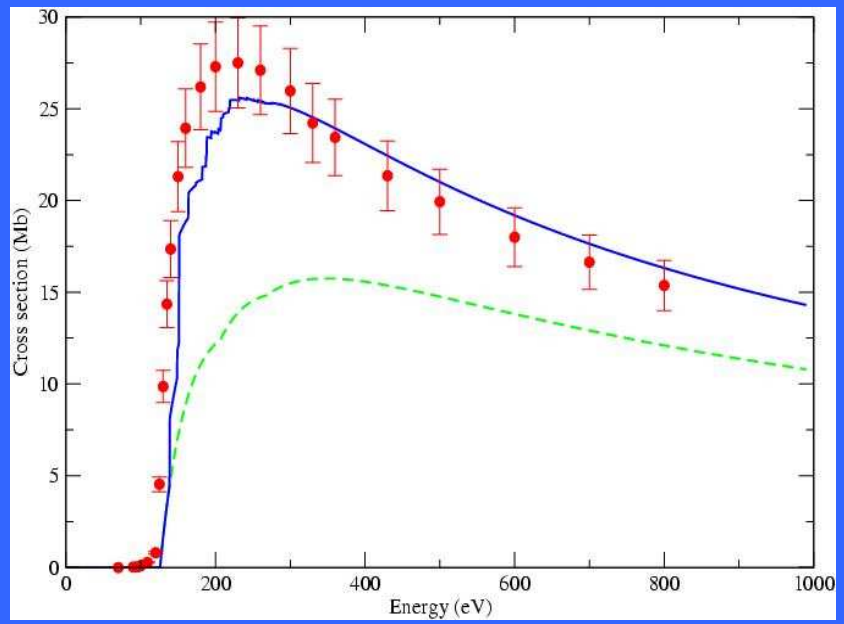
- Various levels of calculation
  - Intermediate coupled distorted-wave (ICDW)
  - LS coupled distorted wave (LSDW)
  - Configuration-average distorted-wave (CADW)
  - Classical Trajectory Monte Carlo (CTMC)



Resonance plot for Cl^{13+} showing the first observation of trielectronic recombination

Other methods "unleashed" by advanced computation and computers : Distorted-wave Born approximation and Classical Trajectory Monte Carlo techniques

- Dielectronic recombination project using ICDW for laboratory and astrophysical elements
  - Li, Be, B, C and O iso-electronic sequences completed
- Benchmark from ion storage ring experiments
  - Cl^{13+}
- Heavy element ionization/recombination using CADW
  - Ar, Kr, Xe, Mo, Hf, Ta, W, Au

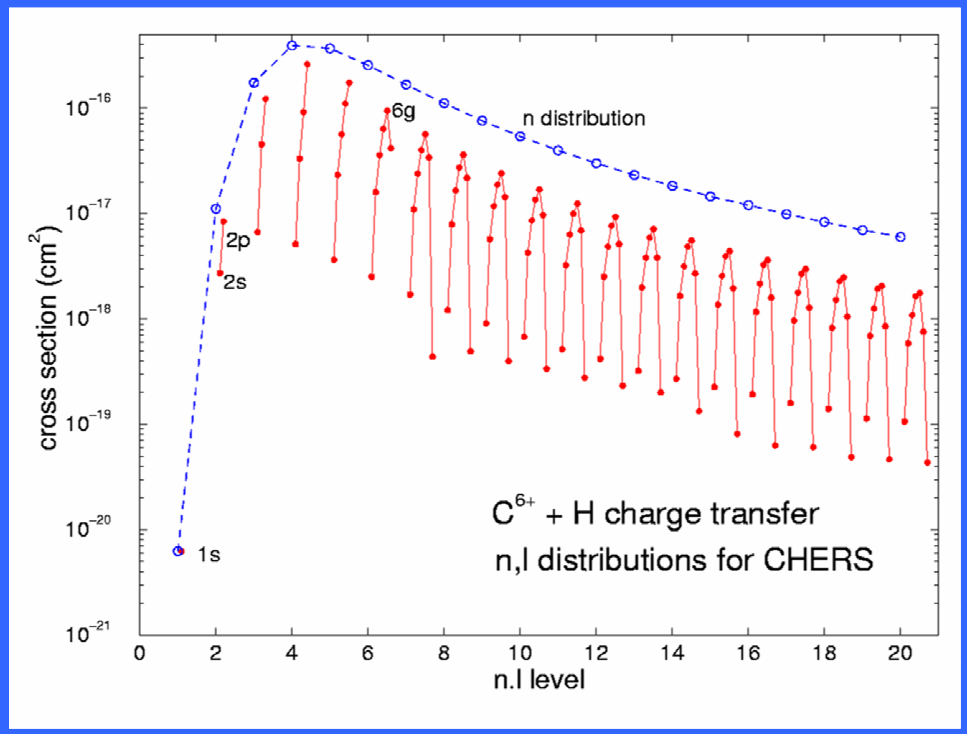


Bi^{7+} $5s^2 5p^6 5d^8$
ionization cross section

Other methods "unleashed" by advanced computation and computers : Distorted-wave Born approximation and Classical Trajectory Monte Carlo techniques

- CTMC calculations for TRANSP, ONETWO beam penetration, stopping, etc. analysis and for CHERS

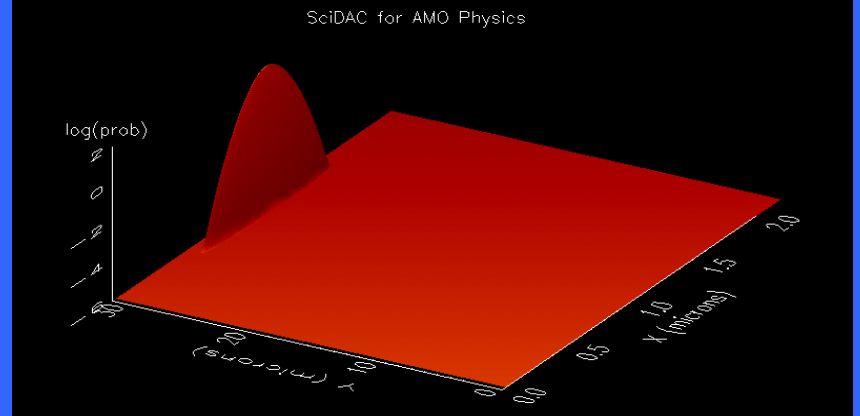
- Excitation, ionization, charge transfer of ions with H and H*



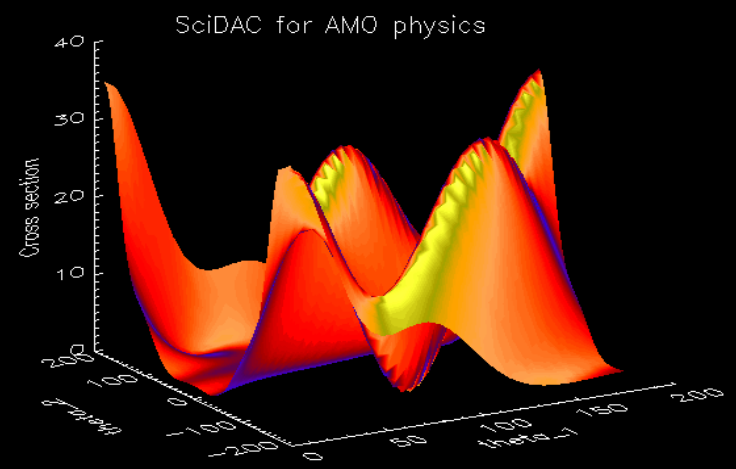
State-selective charge transfer cross sections for major impurity ions and for diagnostic species

Broad Science Spin-offs

- TDCC for
  - (γ,2e) on He, Be, Li+, quantum dots, H_2
  - (2γ,2e) on He
  - (γ,3e) on Li
  - $e^+ + H$
- LTDSE for
  - $p^- + H$, He
  - BEC in fields
- CTMC for
  - e + atoms in ultracold plasmas
  - γ + atoms in high Rydberg states



Propagation of a 2D Bose–Einstein condensate down a harmonic waveguide. Attractive interactions between atoms result in a bright soliton. In support of MIT experiments.



Double photoionization of He – triple differential cross section. The time steps show the energy sharing of the outgoing electrons. In support of synchrotron experiments in the USA and Europe.

Examples of collaborations with laboratories

DIII-D

Li generalised collisional-radiative coefficients used in impurity transport studies

EFDA-JET

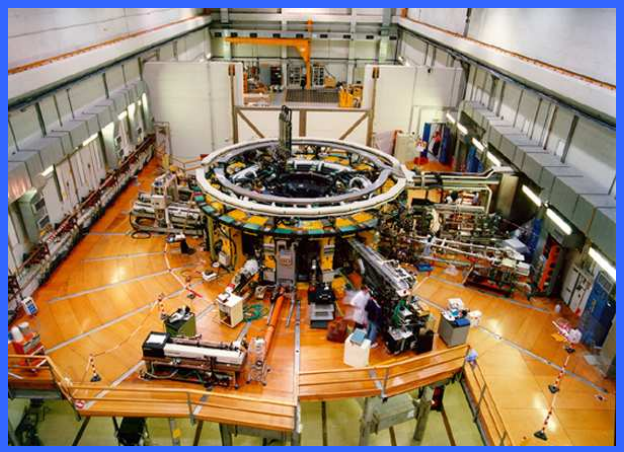
He R-Matrix excitation data used in helium beam studies, and in non-Maxwellian modeling

Examples of collaborations with laboratories

ASDEX-upgrade

Tungsten ionization data to be used in heavy species studies

RFX



Krypton ionization ionization data is being used in plasma transport studies

Some measures of the impact of this SciDAC project

- Development and utilization of state-of-the-art computational atomic physics codes
- Direct service to fusion research programs
- Four graduate students, five postdoctoral fellows – research experience
- Ten Phys. Rev. Lett. publications and about ten total publications per year during the SciDAC project

Conclusions

- Advances in computational technique and in technology have allowed very large-scale, non-perturbative treatment of atomic collision problems
- This has lead to new discoveries in atomic physics and to substantial support of plasma science objectives
- Significant challenges and opportunities remain for discovery as the needs of fusion and the capabilities of new computation together encourage consideration of more complex atomic collisions, systems involving molecules such as hydrocarbons, and plasma-surface interactions