ADASS XXXVI / SHORT TALK

xstar-tools

AI-Assisted Modernization of the XSTAR Photoionization Code

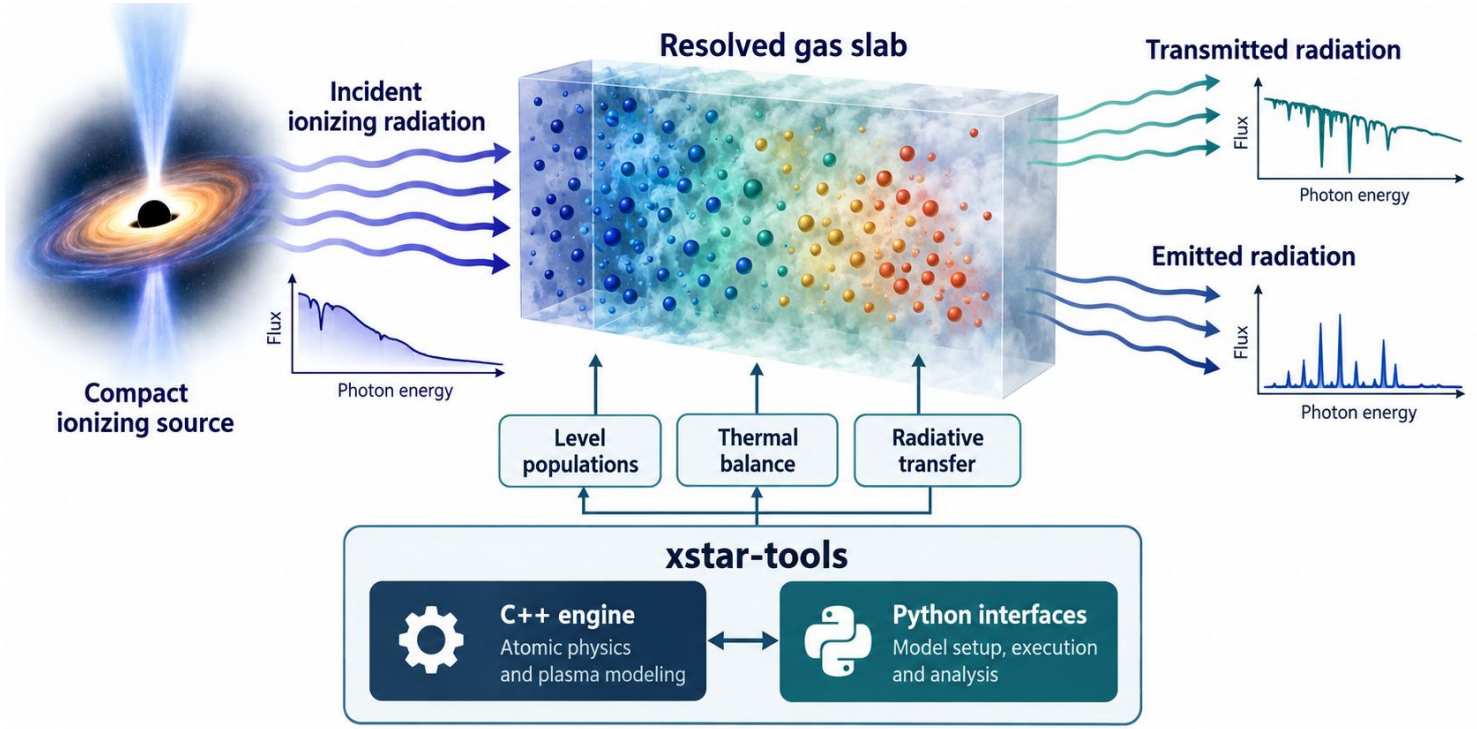
Ash Danehkar

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AI-assisted software · human-led scientific qualification

What XSTAR models

Ionizing radiation interacts with gas and produces spectra.



Independent C++ engine

Scientific model calculations

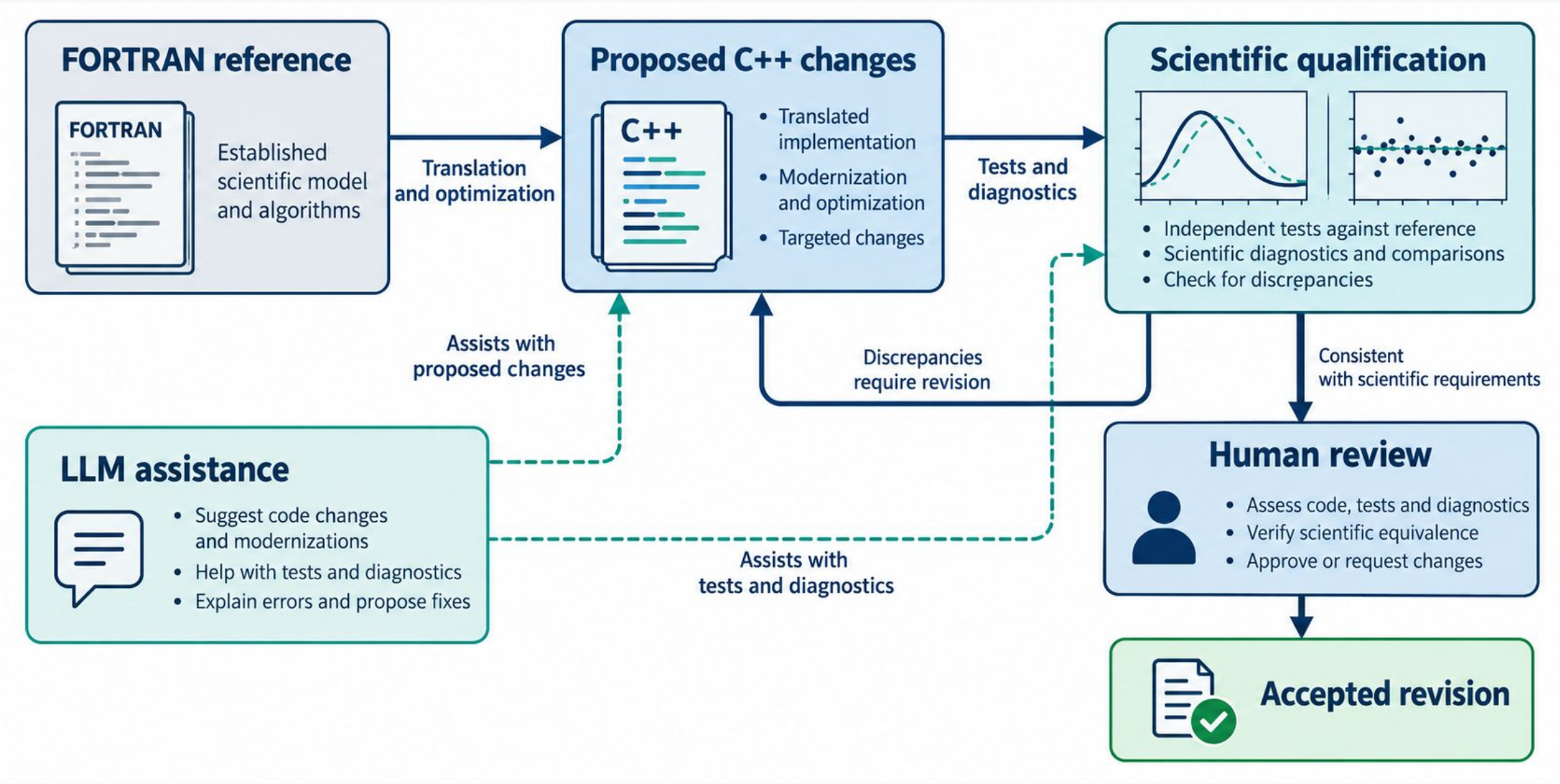
Python interfaces

Model setup, execution and analysis

github.com/xstar-tools/xstar-tools

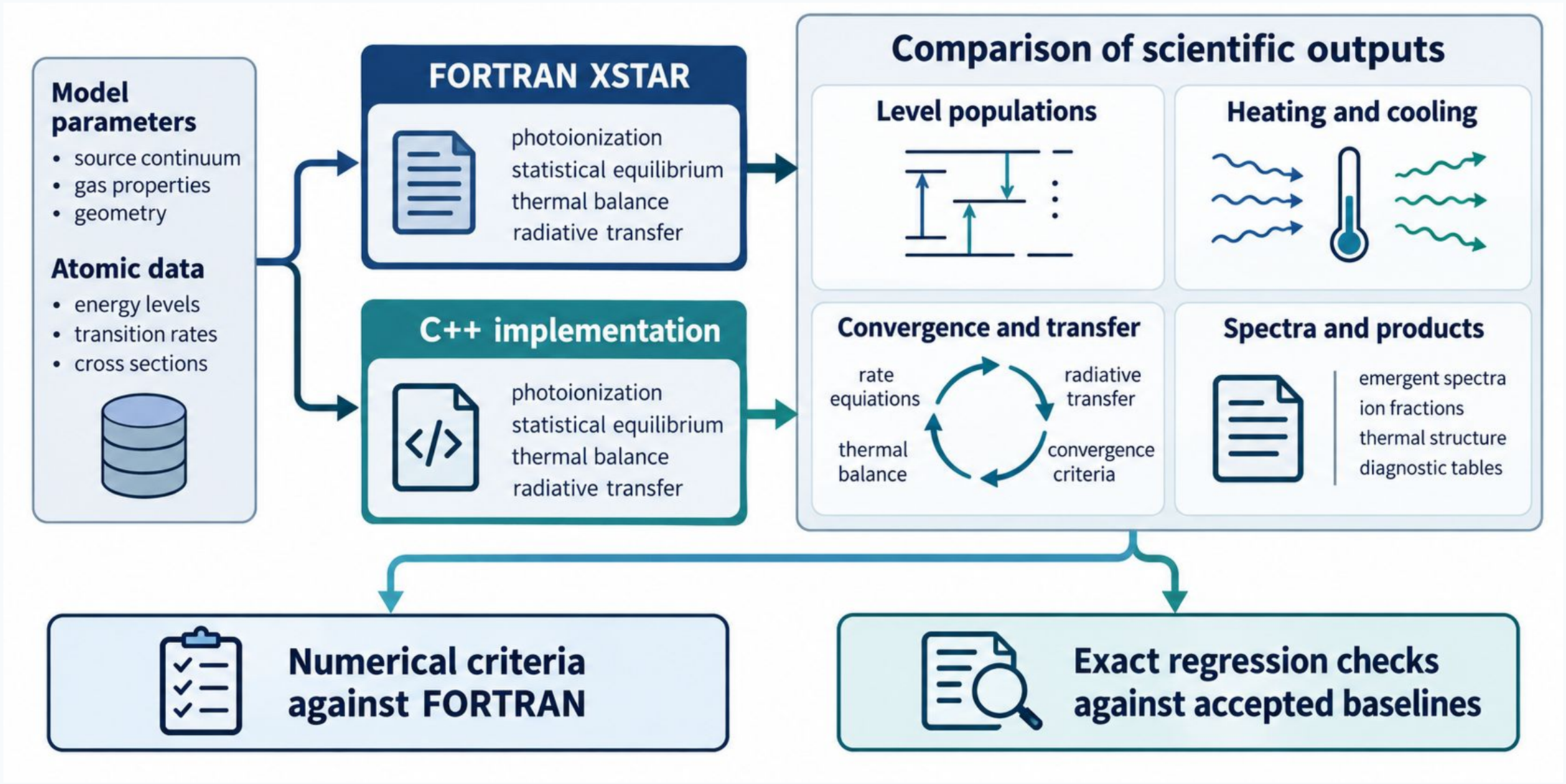
AI-assisted development: a controlled loop

AI proposes changes; tests and human reviewers decide what is accepted.



Scientific qualification is essential

Numerical agreement with FORTRAN and exact C++ regression tests answer different questions.



Compare intermediate states, thermal balance, convergence and spectral outputs

Measured performance improvements

Two distinct historical same-machine comparisons; outcomes depend on the model and host.

EARLIER C++ → OPTIMIZED C++

Historical multi-element test | same HP laptop

≈10× faster than earlier C++

WALL TIME

Earlier C++ ~120 min

Optimized C++ ~12 min

PEAK MEMORY

Earlier C++ ~11–12 GB

Optimized C++ ~3.7 GB

≈ two-thirds reduction in peak memory

FORTRAN XSTAR vs. OPTIMIZED C++

Separate historical test | same ASUS workstation

1.42× faster in this model

WALL TIME

FORTRAN 941 s

Optimized C++ 661 s

PEAK RSS

FORTRAN 2.57 GB

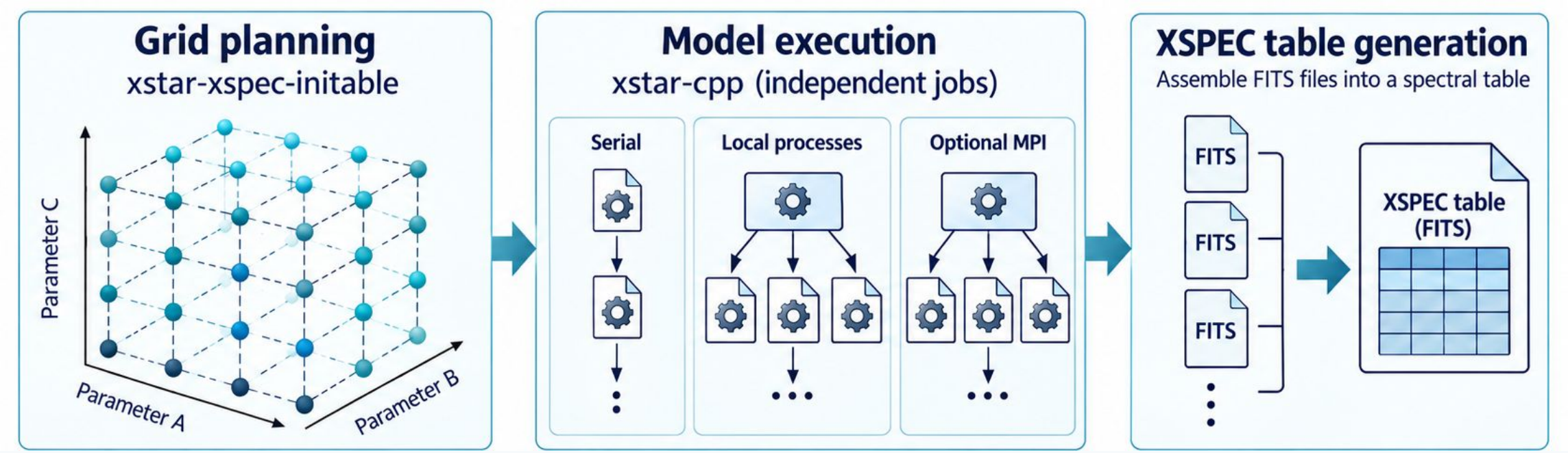
Optimized C++ 3.78 GB

C++ uses more memory in this test

Historical measurements, not repeated statistical benchmarks

Native model grids → XSPEC spectral tables

Plan a grid, run independent models, and collect results in a reproducible order.



MODEL FITS PRODUCTS

Assemble scientific arrays in canonical grid order.

PER-JOB STEP LOGS

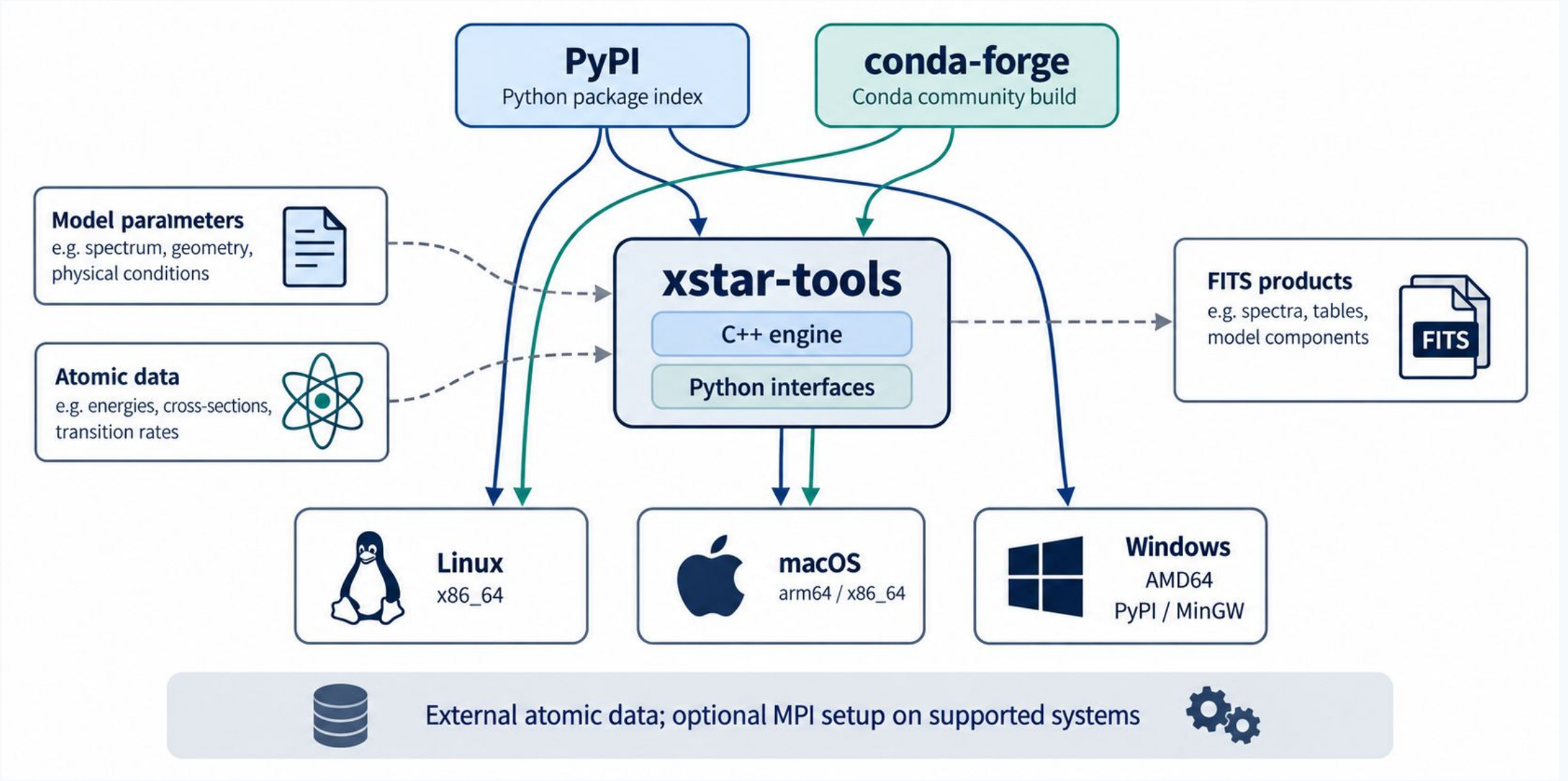
Concatenate logs separately for a traceable run history.

FUTURE EXTENSION

Post-process hydro / MHD simulations for synthetic spectra.

Takeaway: AI can speed up scientific software engineering; qualification and human review protect the science.

Portable software and supported platforms



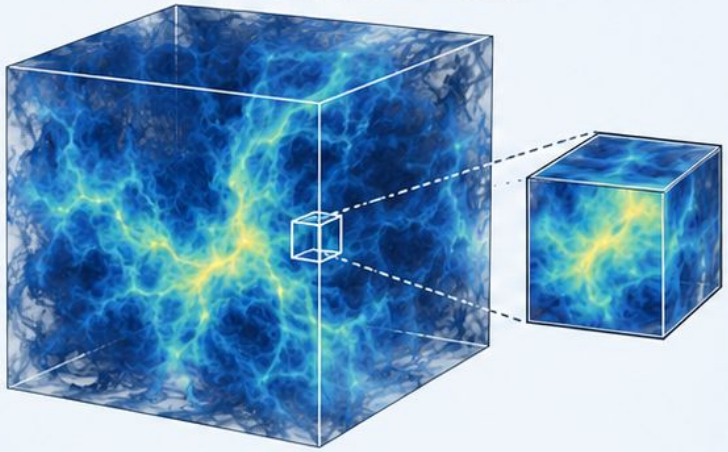
Native builds qualified on Linux, macOS and Windows

Future direction: hydro/MHD post-processing

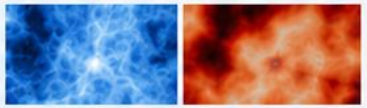
Planned extension: connect MHD simulation conditions to photoionization outputs and synthetic spectra.

Planned development

Simulation fields



Density and temperature

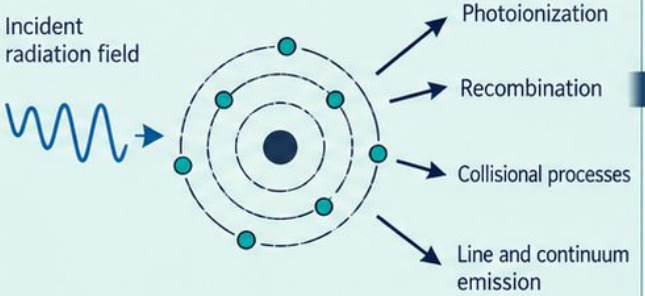


Radiation environment



xstar-tools

Photoionization calculation



Outputs (post-processed cell)

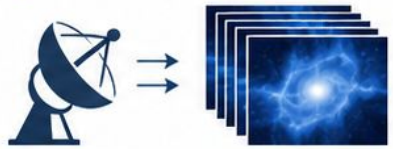
Ion populations



Emissivities and opacities

$j_\nu \ (\lambda, T, n, \ldots)$ $\kappa_\nu \ (\lambda, T, n, \ldots)$

Synthetic observables



Images, spectra, and derived quantities

Reference-based validation



Compare with established atomic data and reference models

- ☑ Ionization balance
- ☑ Level populations
- ☑ Emissivities and opacities
- ☑ Consistency across regimes

Human review



- ☑ Inspect representative cells and outputs
- ☑ Verify physical plausibility
- ☑ Check edge cases and model assumptions
- ☑ Guide iteration and improvements