Jacobian-free Newton Krylov method for multilevel NLTE problems

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Introduction

The calculation of the emerging radiation from a model atmosphere consists in solving the nonlocal thermodynamical equilibrium (NLTE) problem. It is a crucial part of an inversion code and is computationally extensive. The NLTE problem is highly non-local and non-linear and therefore requires iterative solving techniques to be dealt with.

We developed a JFNK solver for this problem, which is based on the Newton-Raphson method. The framework is completed with a Python version of the RH code (Uitenbroek 2001), Ca II and H I atomic models as well as a FAL-C model atmosphere.

Here we investigate the performance of our solvers, with a direct comparison with the robust and well tested Rybicki & Hummer 1992 (RH92) method.

Krylov solvers and JFNK

- The NLTE problem here is about solving the statistical equilibrium and particle conservation equations for the population densities of a atomic species

$$\mathbf{F}(\mathbf{n}) = \begin{cases} \sum_j n_j(C_{ji} + R_{ji}(\mathbf{n})) - n_i \sum_j (C_{ij} + R_{ij}(\mathbf{n})) \\ \sum_j n_j - n_{\text{tot}} \end{cases}$$

and is done by solving $\mathbf{F}(\mathbf{n}) = \mathbf{0}$ with the Newton-Raphson method. $\mathbf{F}$ is the residual vector.

- The Newton-Raphson scheme requires the computation and inversion of Jacobian matrices. We can deal with this extensive process by using a Krylov solver.

- Krylov solvers solve large linear systems iteratively to a specified accuracy. When applied to the Newton-Raphson scheme, they only require Jacobian-vector multiplications which are approximated using finite differences. Hence Krylov solvers only need residual vector estimations, no matrices are built or stored during the solving process. This is JFNK.

Optimal behavior of JFNK?

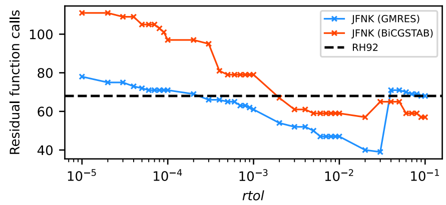

Fig.1 *Residual vector calls required for convergence vs. the Krylov solver relative tolerance for the three-level Ca II setup.*

- High Krylov accuracy: Extra Krylov iterations required. No gain in Newton-Raphson number of iterations.

- Low Krylov accuracy: Fewer Krylov iterations required. Extra Newton-Raphson iterations are required.

- Optimal accuracy: Trade-off between Krylov and Newton-Rahpson number of iterations.

RH92 vs. JFNK

We compared the JFNK and the RH92 solutions both in accuracy and amount of formal solver solutions required to converge. We used two metrics to estimate the accuracy and convergence level of a solver:

- The residual norm $||\mathbf{F}||_\infty$ is directly computed from the residual vector. It is the true error in the rate and conservation equations.

- The population change norm $||\delta\,\mathbf{n}/\bar{\mathbf{n}}||_\infty$ monitors how much the population densities are evolving from a Newton-Raphson iteration to another. It is used as the convergence criterion in most solvers and ours as well.

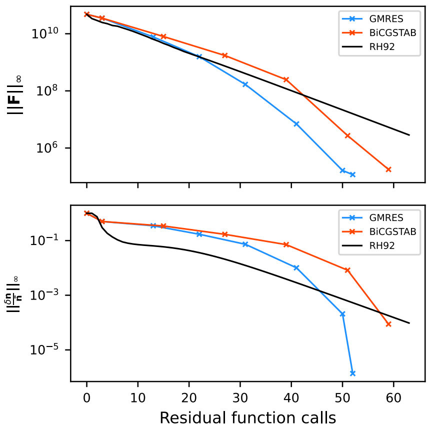

Fig.2 *Residual (Top panel) and population change (Bottom panel) norms during the solving process of the six-level Ca II setup. The initial population densities are the LTE ones. The Krylov relative tolerance is 0.01.*

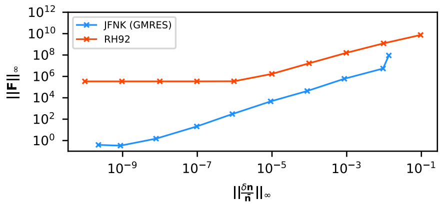

Fig.3 *We ran the different solvers to converge to several convergence levels. For every run, we plot the final reading in* $||\mathbf{F}||_\infty$ *and* $||\delta\,\mathbf{n}/\bar{\mathbf{n}}||_\infty$. *The Krylov relative tolerance is 0.01. Initial population densities: LTE ones. Six-level H I setup.*

We noted:

- JFNK solvers are always more accurate than RH92 for a same level of convergence. Therefore fewer Newton-Raphson iterations are needed to achieve the same accuracy level as RH92.

- JFNK solvers require less formal solutions than RH92 for the Ca II setups.

- The population change norm is not a good convergence indicator.

Emerging spectrum in a non-static atmosphere

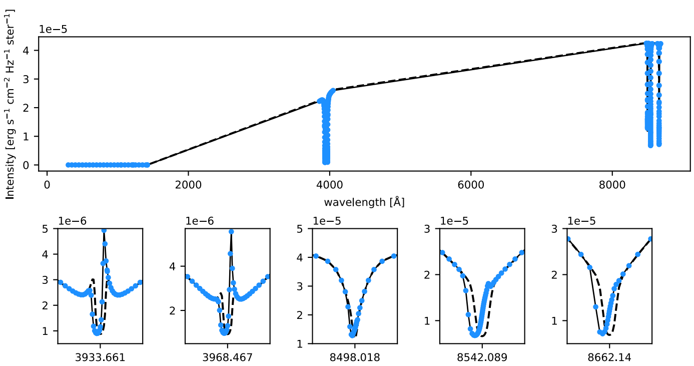

Fig.4 *Emerging spectrum for a FAL-C atmosphere with an artificial sharp velocity gradient at the lower chromosphere and the six-level Ca II setup. Initial population densities: LTE ones. Krylov relative tolerance is 0.01. Solid line: RH92 output. Blue dots: JFNK output. Dashed line: static atmosphere solution.*

Conclusion

The preliminary investigation of the JFNK method applied to the NLTE problem is very promising. The solvers we developed converge twice as fast as RH92 in the best cases. The JFNK solvers can deal with most physics effects due to their flexibility (e.g. velocity gradients, PRD, polarization) and can be further upgraded to improve their performances. A downside of the method is a potential failure for certain initial population densities as a Newton-based method. Furthermore, the optimal Krylov relative tolerance is problem dependent.

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