

Spectroscopic and polarimetric inversions: Our key to unlocking the secrets of the solar atmosphere

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Synopsis

Advances in our understanding of the Sun will require the accurate and consistent measurement of the physical conditions in different regions of the solar atmosphere. The richest information, encoding the full state integrated over of the atmospheric volume in which they are formed, is contained in the detailed shapes of the numerous spectral lines present in the solar spectrum. But this integration along the line of sight is highly non-linear, which means that inferring the true physical conditions requires solving a complicated, ill-posed inverse problem. This challenge is being addressed through powerful codes that treat ever more complex aspects of the solar atmosphere - the breakdown of local thermodynamic equilibrium (or non-LTE), non-equilibrium hydrogen ionization, deviations from hydrostatic equilibrium, and multiple methods of deriving chromospheric and coronal magnetic fields. However, to reach the full potential of these techniques, the community must make a concerted, sizable effort to improve and enhance them, both in terms of their physical veracity as well as their computational tractability. These methods will be essential for fully exploiting the data from new and proposed solar facilities or missions. Reliable outputs from inversions will be a key component of more realistic extrapolations of the magnetic field of active regions and the heliosphere. These inversion methods, if accurate and robust, can become a key tool in determining the structure of stellar atmospheres, but will also become crucial for the operational prediction of the energetics of the Sun's magnetic field and the driving of space weather and changes in the solar spectral irradiance.

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Introduction

Modern studies of the solar atmosphere rely on the accurate and consistent inference of the physical conditions therein. As it is impossible (or impractical) to directly measure these conditions in situ, solar physicists use remote sensing to infer information about the physical conditions in the solar atmosphere from the emitted electromagnetic radiation (light). Spectral lines are especially rich in their diagnostic content since the atomic (or in some cases molecular) transitions are sensitive to a variety of physical phenomena that encode additional information about their local or nearby environment, including velocities (through Doppler shift) and magnetic fields (through Zeeman and Hanle effects). Spectral lines are sensitive to a range of depths in the solar atmosphere (top panel in Fig. 1) and thus are the result of an integration over our line-of-sight, with multiple components and non-linear combinations of physical parameters that come into play. A computational approach to disentangling these contributions and mapping the observed spectrum to a collection of depth dependent physical parameters is called a spectroscopic (or spectropolarimetric) inversion.

This inversion process iteratively finds a model atmosphere that produces a synthetic spectrum (through a formal radiative transfer calculation) that best matches the observed (polarized) spectrum, while taking into account the relevant microscopic processes (chemical equilibrium, ionization, excitation, absorption, and emission). Such techniques have become a mainstay of modern solar physics research, and are applied from the photosphere to the corona. Exactly because they are crucial to future progress in the field, it is imperative that these inversion outputs, as well as the methods (codes) themselves, be as accurate, reliable, and broadly available as possible. Advances in theoretical understanding of radiative transfer, improvements in computing resources, leveraging of 3D radiative magnetohydrodynamic (rMHD) simulations, and community efforts in developing and distributing efficient inversion codes have enabled new ways to understand the Sun on different temporal and spatial scales. By witnessing the extent that these techniques have already provided us with a deeper understanding, we can envision many ways that we can build on them, to address new classes of problems.

In this whitepaper, we present some current applications of these techniques, outline some of the known needed improvements to build on this heritage, and highlight the institutional support that will be necessary to ensure the power of these methods will be widely available in the community to invigorate studies using the wealth and breadth of solar observations.

Current Situation

Photospheric vector magnetic fields have been routinely inferred from ground-based observations for decades. The most common approach has been to use schemes based on the Milne-Eddington (ME) approximation, which simplifies the inversion problem by

assuming physical conditions are constant over the formation region of the line. This allows this algorithm to be implemented into data pipelines and applied automatically on continuous, high volume, data streams to infer, among other things, the magnetic field vector in the Sun's photosphere (e.g. SDO/HMI, Scherrer et al., 2012; Borrero et al., 2011; Centeno et al., 2014; Hinode/SP, Kosugi et al., 2007; Lites et al., 2013). In fact, the method is robust enough that the Polarimetric and Helioseismic Imager (PHI) instrument on Solar Orbiter (Solanki et al., 2020) was designed to perform this inversion process onboard in interplanetary space, downlinking only the recovered atmospheric parameters to Earth (Albert et al., 2020).

The stringent assumptions that go into the ME approximation, however, limit its applicability to low photospheric lines, and simple, perhaps unrealistic, models of the solar atmosphere. More sophisticated inversion approaches become necessary as we move to higher, less-dense regions of the atmosphere. A major goal is that of achieving the same level of reliability and robustness of ME methods even with codes that incorporate the significant additional complexity and computational costs needed to treat the inversion problem beyond the low photosphere.

In the chromosphere, where the magnetic field signatures are significantly weaker, rigorous diagnostics are even harder. The only attempt at a near-real-time data pipeline has been made with SOLIS data (Jin et al., 2013), applying the very restrictive assumption of the Weak Field Approximation (WFA). This approach provides rough estimates for the vector magnetic field, but does not ascribe them to specific geometric heights, nor can it infer depth variation of the field. Proper interpretation of chromospheric profiles instead requires calculations of level populations that are not controlled solely by collisional processes but also by the non-local radiation field (the so-called non-LTE condition, or NLTE), among other complications, discussed below. Sophisticated chromospheric inversion packages have been developed (Socas-Navarro et al., 2015; Milic and van Noort, 2018; de la Cruz Rodríguez et al., 2019; Ruiz Cobo et al., 2022) but they are computationally prohibitive for routine application to large data volumes and often require fine-tuning by experienced users.

Nevertheless, there have been significant advances in fundamental chromospheric science enabled by state-of-the-art inversions applied to high-resolution observations, for example in evaluating the role of magnetic fields in the heating of the quiet Sun chromosphere through ubiquitous magnetic flux cancellation events (Gošić et al., 2018), in inferring the stratification of the atmosphere undergoing magnetic reconnection (Vissers et al., 2019; Díaz Baso et al., 2021), in constraining heating rates due to emerging magnetic flux in an active region (da Silva Santos et al., 2022), in assessing the role of Alfvén waves and ion-neutral effects in plage heating (Anan et al., 2021), and in constraining temperatures of off-limb solar structures such as prominences (Jejčić et al., 2022) and spicules (Kuridze et al., 2021).

Accurately measuring the magnetic field in the chromosphere is crucial for understanding this region's intricate fine-scale structure and complex dynamics over a range of spatial scales, as well as comprehending the nature of chromospheric heating and its possible relation to coronal heating (e.g., Carlsson et al., 2019). Doing so will ultimately require acquiring multi-wavelength data sets and robust inversion codes that necessarily need to incorporate more physical realism (e.g. Hanle effect, non-LTE ionization) while still being able to cope with ever-increasing data volumes.

Moving even higher in the atmosphere, inversions of the coronal emission line profiles are still at an early stage, due in part to fundamental observational challenges, but also due to issues with poorly known atomic parameters for the highly ionized species and the difficulty of interpreting measurements potentially integrating over many optical thin features along the line of sight. Several authors have explored complexities that bedevil coronal inversions, such as degeneracies, lack of disambiguation methods, and symmetry-breaking effects (e.g. Schad and Dima, 2021). Several prototype inversion methods are being explored, including analytical inversions (Dima and Schad, 2020) and the forward-model-comparison of the Coronal Line Emission DataBase (CLEDB) method (Paraschiv and Judge, 2022).

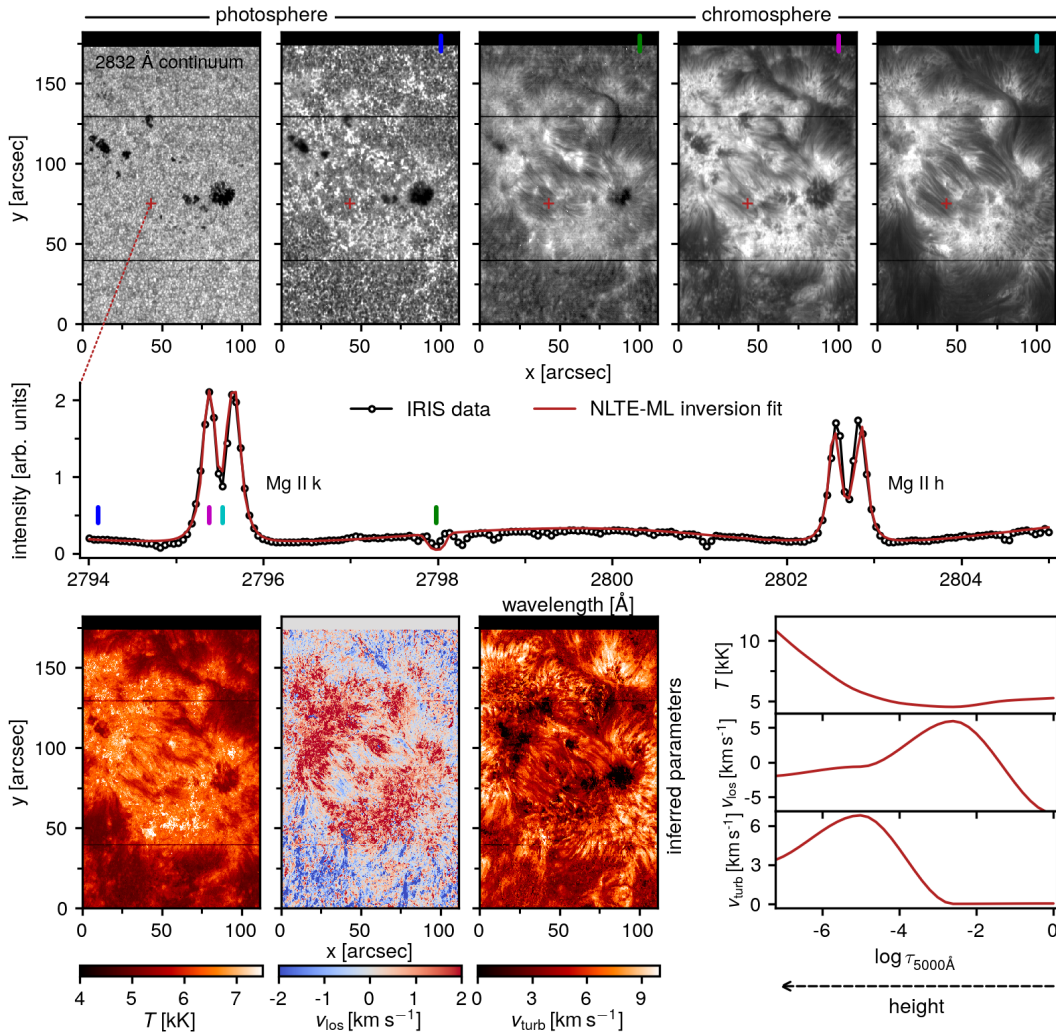


Fig. 1 - NLTE inversions of spectroscopic data taken by NASA's IRIS UV satellite using a machine learning code (IRIS²). The top row panels show an active region at different wavelengths within the Mg II k line, sampling from the photosphere to the upper chromosphere. The middle panel shows an example spectrum (black circles) and the best model fit (red line); the small vertical lines show the wavelengths displayed in the upper panels. The bottom row shows the inferred (height-averaged) chromospheric temperatures, line of sight velocities, and microturbulence (left panels) and the stratification of those parameters as function of optical depth (right panels) for the example fit.

Necessary Advances

1. Chromospheric magnetic fields

The measurement of chromospheric magnetic fields is challenging both from the observational and the theoretical perspectives. On the one hand, chromospheric fields are weaker than their photospheric counterparts, imprinting typically smaller polarization signals in spectral lines. Measuring these signatures with adequate signal-to-noise ratio requires very sensitive instruments and highly accurate calibration methods, as realized, for example, by the Daniel K Inouye Solar Telescope (DKIST; Rimmele et al., 2020). On the other hand, interpreting the polarized radiation with the goal of inferring the magnetic field relies on our ability to model the subtle quantum-mechanical processes that generate and modify polarization in chromospheric lines. This is a computationally arduous task marred by many degeneracies, resulting in a highly ill-posed inverse problem that often seems intractable. However, having reliable ways to determine the chromospheric field is key for constraining the mechanisms responsible for chromospheric heating as well as quantifying the lower magnetic boundary for coronal field extrapolations (see, for instance, the review by Lagg et al., 2017). The latter is of particular relevance to the extrapolation of polar fields into the heliosphere, where photospheric “measurements” of net flux at the solar poles differ by a factor of 2-5 with respect to the in-situ measurements at L1 (Linker et al., 2017).

2. Joint analysis of Hanle and Zeeman effects

While the Zeeman effect is the dominant source of spectral line polarization in the photosphere, scattering polarization can be important for some lines and especially in the chromosphere and corona, where most lines show signatures of the joint actions of the Hanle and Zeeman effects. The Hanle effect is widely used in the diagnostics of prominence and filament magnetic fields, using simple models (e.g. Orozco Suárez et al., 2015) but only a small subset of the solar physics community is currently focusing on its diagnostic potential in the overall chromosphere (and also for certain photospheric lines, for example the Sr I 4607; see Zeuner et al., 2020, 2022). Interpreting Hanle signatures in photospheric and chromospheric spectral lines however might prove to be crucial, as it provides us sensitivity to weak, mixed-polarity fields on the sub-pixel scales that are completely invisible to the Zeeman effect. Still, interpretation of scattering polarization signatures and their modification via the Hanle effect poses significant challenges, stemming from the theoretical complexity and the high computational cost of their modeling (Štěpán and Trujillo Bueno, 2013; del Pino Alemán et al., 2016). For example, the newly developed Tenerife Inversion Code (TIC, Li et al., 2022) is an advanced tool to extract weak chromospheric magnetic fields generated in this regime, but does so at large computational expense (the inference from a single Mg II h+k Stokes spectrum uses ~ 1000 core-hours). Development of robust and user-friendly methods and efforts of the wider community, likely combined with the machine learning approaches, are therefore necessary to make use of these complementary diagnostics in weak field regimes.

3. Coronal magnetic fields

Coronal magnetic fields have been problematic to measure, as current instrumentation hardly provides enough information to produce meaningful inversions. Production of vector magnetic maps of the corona is the long-term goal, and the capability to measure magnetic fields via full Stokes polarimetry of the corona is imminent with new-generation facilities like DKIST, UCoMP, and the future COSMO observatory (see WP by Tomczyk et al.) going into operations. These new observations will enable the community to directly probe magnetic fields in the higher atmosphere of the Sun, without relying on the drastic limitations and inaccuracies that hinder extrapolations.

Several methods to derive coronal magnetic fields have for now been tested mostly on models and the scarce coronal observations, for example tomography (Kramar et al., 2016) or global magnetic fields constrained by linear polarized coronal data and photospheric magnetograms. Another approach proposes probing magnetic structures indirectly by using Alfvén wave propagation to infer plane-of-the-sky (POS) magnetic fields in the solar corona, from linear-polarization observations and Doppler oscillations (Tomczyk et al., 2007; Morton et al., 2016; Yang et al., 2020). Full polarimetric inversions like the analytical inversion of Dima and Schad (2020) or the forward model comparison CLEDB inversion (Paraschiv and Judge, 2022) are under development, with the goal of using all the information from single or dual line observations to infer the full vector magnetic fields under distinct sets of assumptions. Currently, all polarimetric methodologies are subject to degeneracies, and suitable disambiguation methods have not yet been developed. Devising an inversion method that leverages both polarization and velocity information appears promising and a goal to be implemented in the coming year. The availability of multi-vantage-point observations from Solar Orbiter over the coming decade will allow critical testing of new and robust inversion and disambiguation schemes.

4. Physical Veracity

A multitude of higher order physical plasma effects, which have been found to be important in the forward modeling of the solar atmosphere, have not yet been implemented in current spectral inversions. For example, time dependent non-LTE hydrogen ionization balance due to the long recombination time scales has been long known to be important in the chromosphere (Kneer, 1980; Carlsson and Stein, 2002). This effect leads to significantly higher electron densities than predicted from statistical equilibrium calculations, which cannot be inferred robustly from current inversions. These effects are important for the interpretation of diagnostics which are very sensitive to electron densities, such as mm-continua (Hofmann et al., 2022). Even accounting for a time-independent non-LTE ionization is computationally demanding as it increases computing time by a factor of four or more. Another major problem with current inversions is the fact that they retrieve an atmosphere on optical depth scale, not physical height. This is because the spectrum is completely insensitive to the vertical displacement of the atmosphere underlying the observed pixel. Aligning resulting atmospheres in optical depth is a very non-trivial task, leading to significant challenges in interpreting observations with high spatial resolution and using the inversion outputs in data assimilation tasks (see item 7). A related limitation of inversions is the necessity of assuming that the atmosphere is in hydrostatic equilibrium, in order to eliminate gas pressure as a model parameter and thus increase their robustness

(for the discussion of this effect as well as the geometrical height inference, see Borrero et al., 2019). Finally, multidimensional, non-LTE radiative transfer effects (i.e. lateral scattering of photons in the solar atmosphere) have been shown to be important for the proper modeling of spectral lines, especially in the chromosphere (Bjørgen et al., 2019, Štěpán and Trujillo Bueno, 2016). Efforts in spatially coupled, multidimensional inversions are a logical, but imposing, step toward improving the veracity of inversion techniques (Štěpán et al., 2022).

5. Code Reliability

The physical state of the Sun's atmosphere derived through spectral line inversions is an inference, not a direct measurement. The quality and robustness of this inference depends on many different aspects of the observations themselves (including photon noise, polarimetric sensitivity, spatial, temporal and spectral resolution, etc), as well as the forward modeling assumptions (both in the radiative transfer calculation and the instrumental model) that drive the inversion algorithm itself. All of these will result in uncertainties in the retrieved physical quantities (see, e.g. Gosain, 2017), which are imprecise at best, and wildly inaccurate in the worst case scenarios. Systematic biases resulting from spectral line assumptions are often unknown (or unaccounted for), which can lead to incorrect conclusions about the Sun's physical state and evolution. More effort and resources should be devoted to quantifying the biases and limitations of different inversion methods in order to provide usable uncertainties along with the inversion results to the solar community. The primary means to check the accuracy and reliability of the inversion codes is to perform forward modeling tests based on the rMHD numerical simulations, followed by the inversion of the obtained synthetic profiles. The comparison of the original and inferred quantities helps quantify biases and reliability of different inference methods (e.g. da Silva Santos et al., 2018; Milić et al., 2019; Centeno et al., 2021). To enhance and streamline this process, the simulations, synthetic profiles and observational model (atmosphere, telescope, and instrument) should be packaged as a coherent dataset that can be used for different experimental needs.

6. Inversion Efficiency

An inversion calculation involves multiple evaluations of the emergent spectrum, which, in turn, requires solution of nonlinear systems of equations, integration of partial differential equations or even iterative solution of the non-LTE problem. This makes them extremely numerically demanding. Even a very optimized non-LTE inversion code (e.g. DeSIRE, Ruiz Cobo et al., 2022) requires on order of 10s per spectrum to recover the atmospheric structure. Inverting a 2000×2000 pixel map would thus require a million CPU hours: a substantial cost in time and resources, as well as a non-negligible contributor to climate change. Increasing the efficiency of the inversion codes is thus paramount for progress and efficient use of the upcoming large datasets.

Machine learning (ML) approaches, and specifically Deep neural networks (DNNs) vastly accelerate the inversion process by approximating the mapping between the observed (polarized) spectrum and the structure of the underlying atmosphere. This mapping is based on a learning process using an application-specific training data set, produced either from MHD simulations (Asensio Ramos and Díaz Baso, 2019; Osborne et

al., 2019) or from the results of conventional inversions (Sainz Dalda et al., 2019; Milić and Gafeira, 2020). Once trained, ML methods are extremely efficient to apply to new data and offer a speed increase of several orders of magnitude. Figure 1 shows such an example: an active region was observed by IRIS in the Mg II h and k lines, probing a wide range of heights from the photosphere to the upper chromosphere (top panels), and the spectral lines inverted by the IRIS² method of Sainz Dalda et al (2019). IRIS² matches model atmospheres for the whole FOV, more than 175,000 spectra, in about 143 s on a single laptop CPU, providing spatial and temporal maps of parameters, such as temperature, line-of-sight velocity, and microturbulence (bottom panels). An equivalent inversion using the STiC inversion code (de la Cruz Rodríguez et al., 2019) would take 10^5 times longer.

Once a neural network with a suitable architecture (or another ML method) can be trained using a sufficiently large or complete training data set to account for the natural variation of the solar atmosphere, from quiet to active conditions, there will not be a need to perform the explicit inversion process for any subsequent observations of comparable solar structures using the same spectral diagnostics. This approach requires significant human and computational resources to validate and optimize, following the same forward - backward approach outlined in section 5, before it can be converted into a pipeline available to the solar community. Ultimately, this would vastly reduce the computational and ecological burden of inversions. The atmospheres returned from the ML approach, however, are only as reliable and diverse as the input atmospheres, which places an additional challenge to have more realistic rMHD simulations.

7. Data Driven/ Data Assimilation Modeling

Solar active regions (ARs), which harbor strong magnetic fields, are the source of eruptive and transient phenomena, for example, flares, CMEs, jets. etc. These events often originate at coronal heights, where the magnetic energy is stored in complex magnetic structures, but they affect different layers of the solar atmosphere almost simultaneously. Even though the coronal magnetic fields are weaker than in the lower atmosphere, they govern all the dynamics of the coronal plasma above ARs. Since direct measurements of the coronal field are quite limited, and lack sufficient spatial or temporal resolution, current coronal magnetic models mostly rely on the data-driven simulations based on the photospheric magnetograms as boundary conditions. In the data-driven modeling, time sequences of photospheric magnetograms are provided as boundary data and changes are made to the coronal magnetic field in response to photospheric changes such as shearing flows, flux emergence etc. (Cheung and DeRosa, 2012; Hoeksema et al., 2020). Such models also allow us to derive the 3D time-dependent quantities such as electric current, Poynting flux, and the magnetic field topology. Importantly, these models facilitate our understanding of energy transfer from the photosphere into the chromosphere and corona, and capture important dynamical processes during transient events like flares and CMEs.

As the data-driven models rely highly on the accuracy of the vector magnetogram, it is essential to develop inversion tools that can provide fast and accurate vector magnetograms in the photosphere and the chromosphere. ME inversion is the simplest, fast, and widely used approach to infer the magnetic field vector in the photosphere but fast, consistent and reliable inference of the vector field in the chromosphere is key to perform data-driven simulations or magnetic field extrapolations from multiple heights (Yelles Chaouche et al., 2012; Yadav et al., 2019).

Development Framework

With a concerted effort to make progress on the improvements described above, we can realize the full promise of these spectropolarimetric inversion techniques over the coming decade. This will enable the community to perform innovative science using the wealth of solar data that will be available from a variety of facilities and missions. However, because of the scope and interconnectedness of these challenges, achieving these advances will require a more structured approach than previous efforts. These efforts based on computational work, requiring focused software development, are scientific studies in their own right, and as fundamental to advancing knowledge as instrumental or theoretical studies. We thus recommend the establishment of a funding scheme promoting team collaborations, and the establishment of hubs for coordinated research, such as NASA DRIVE Science Centers or NSF Science and Technology Centers, that will bring together researchers with different backgrounds (observational, modeling, computer science, etc.) to concentrate efforts on some key problem areas. ***We envision that these essential efforts should be carried out by at least two science and technology centers, at a cost of \$3-4M per year each, with a lifetime of five years. This will provide the human and computational resources necessary to fully exploit the potential of these spectroscopic inversion techniques to deeply reveal the workings of the solar atmosphere.*** The development of these new techniques should initially be research driven, targeting specific scientific questions that will directly push the boundaries of our physical models and computational capabilities. Some of these development targets should also be designed in consultation with major projects (such as DKIST, MUSE, ngGONG, COSMO, and FASR) so that the inversion methods will support the full exploitation of the data from these projects. As the reliability and efficiency of the inversion process improves, certain methods or algorithms should be actively identified that could support operational needs related to event prediction and space weather forecasting. One key example would be developing the capability to perform coronal and heliospheric field extrapolations that are based on direct measurements of the (force-free) vector magnetic field in the chromosphere.

A concerted effort must also be made to ensure that the techniques that are developed are quickly made available to the full solar community, comparable to the expectations for data availability from a new instrument. This allows all members of the community to equally profit from the implementation of these powerful tools. It is also true that some of the necessary inversion methods might not be in reach of all potential users, because of limitations on computational resources, or the lack of necessary experience in running the more complex codes. In this case, a more desirable and efficient approach would be to provide the inversion output datasets (Level 2) directly to the users, rather than simply the calibrated data (Level 1) and inversion software. Funding should also be provided by the national agencies to support community training and outreach to create an engaged user base, well informed about the potential and limitations of these methods. These efforts should also involve members of the space weather community, to understand other usage opportunities for spectroscopic inversion techniques and foster the transition of these methods to operational applications (R20).

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