Session IV

Chemical Abundances Constraints on Mass Assembly and Star Formation

1 - Modelling the Stars
Are “realistic” model atmospheres realistic enough?

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Abstract. During the latest decades the number of papers on stellar chemical abundances has increased dramatically. This is basically reflecting the very great achievements in telescope- and spectrometer-construction technology. The analysis of the resulting stellar spectra, however, is still not up to the standard that is offered by the observational methods. Recent significant advances in the analysis methods (i.e., in constructing model atmospheres and model spectra to compare with the observed ones) is reviewed with the emphasis on the application to abundance analysis of late-type stars. It is found that the very considerable progress that have been made beyond mixing-length convection and LTE is a major break-through for physically consistent modeling. Still, however, further steps must be taken, in particular for the cooler stars, before the situation is fully satisfactory.

Keywords. stars: atmospheres, stars: abundances, chemical analysis, model atmospheres

1. Introduction

Since the first stellar abundances were derived from model atmospheres many decades ago, the question has been repeatedly asked whether such models have been accurate enough for the purpose. Model atmospheres may be used for various purposes: to describe and further explore the physics of the atmospheres themselves, to reproduce the stellar spectra and other observables quantitatively with few (if any) free parameters, or to solve the inverse spectral-analysis problem, i.e. to deduce the stellar fundamental parameters like $T_{\text{eff}}$, $\log g$, and the array of elemental abundances from the spectra, supplemented with additional observational information like colours, parallaxes and angular diameters. The question to answer in this latter case is then: how accurate will the abundance determinations be, in view of the lack of realism in the models? And, with a specified and required accuracy: what steps need to be taken in constructing the models in order to ascertain this accuracy? In this short review I shall thus neglect the fact that other circumstances, that may often seem more trivial but are sometimes nevertheless quite difficult to deal with in practice, like continuum definition in noisy or crowded spectra, blends, or uncertain $gf$-values, may be sources of error as important as the model atmospheres.

Since the modeling situation for stellar atmospheres and their spectra is widely varying along the spectral sequence, I shall divide the discussion into several parts, starting with solar-type stars and then move towards the cool end of the HR diagram. I shall not cover the early-type stars here, due to lack of space and expertise. Before entering into this discussion, I shall however make a few bibliographic comments.
2. The abundance of abundance papers

From the SAO/NASA Astrophysics Data System (ADS) one may find that the number of published articles with the word abundance in the abstract has increased steadily from about 20 per year in the early 1950s to about 4000 per year at present. This growth seems significantly more rapid than the growth of the number of astronomers – the number of IAU members has increased from about 600 to about 10,000 in the same period. Although a fraction of these papers deal with chemical abundances in non-stellar astronomical objects, or non-chemical abundances, the vast majority of them discuss spectroscopic or photometric estimates of stellar chemical abundances. Altogether, there are more than 80,000 papers published until now on abundances (in this sense). More than half of them were published during the latest decade! It should also be noted that many of these papers nowadays give results for large samples of stars each. The papers constitute about 25% of the number of papers with stars in the abstract. This vast increase of abundance work certainly reflects the advances in telescope design and spectroscopic and detector technology during the period, but also reflects the much improved and automatized methodologies in the analysis of spectra. Some 50 years ago, a PhD thesis could contain a “detailed abundance analysis” of one single star. Now, such – or more refined – analyses are routinely carried out for samples of hundreds of stars.

A similar search for the word abundances + model atmospheres in the ADS abstracts results presently in typically about 300 papers per year. There was a strong increase of such papers, from about ten in the mid 1960s to about 100 in the mid 1970s. At least partly, this seems to reflect the construction of vast grids of non-gray model atmospheres in those years. The leveling off of this increase after 1980 is probably a natural consequence of that model-atmosphere analyses then became standard and were not considered worth explicit mentioning in an abstract.

Searching further in the abstracts we find, somewhat disappointedly, that only about 3-5% of the papers with abundances also include the word errors in their abstracts. Although the abundance papers in general most often give error bars on abundance estimates, the errors as such are obviously not at focus. This is somewhat astonishing since the situation is indeed challenging – while modern spectrometers delivering equivalent widths and other abundance measures to accuracies approaching a few percent for thousands of stars, many of them fainter than 13th, and these small errors for weak spectral features should imply similarly small errors in the abundances, any comparison between reasonably independent determinations show errors that are at least one order of magnitude larger. Yet, among the sources of model errors, shortcomings of the LTE hypothesis, almost always adopted in the model atmospheres of late-type stars and in most cases also adopted at the calculation of spectra, is nowadays explicitly mentioned in the abstracts of about as much as 100 annual papers on abundances which indicates an increasing ability to relax this assumption. The assumption of 1D geometry is also beginning to be relaxed, as is demonstrated by a rapid growth during the last 10 years in the number of abstracts with abundances + 3D models, from practically nothing to presently about 30 papers annually.

3. The basic assumptions

The basic assumptions usually made when standard stellar model atmospheres are to be constructed are usually listed as (1) 1D stratification (either plane-parallel or spherically symmetric geometry), (2) hydrostatic equilibrium, (3) LTE and (4) MLT, Mixing-Length “Theory” convection. When these assumptions are nowadays being relaxed it is
Realistic model atmospheres?

Certainly not a straight-forward process. As the application of MLT is replaced by solving the full hydrodynamic equations, one must see to it that all relevant spatial and temporal scales are taken into account in the simulations. So that the photospheric convective energy transfer, the thermal inhomogeneities and the velocity fields are properly described. This is difficult to do from first principles; instead comparison to detailed observations are necessary in order to ascertain that the range of scales chosen to represent numerically are sufficient. If the LTE assumption is fully relaxed, thousands (or millions!) of new and to a great extent unknown physical quantities, notably cross-sections for inelastic collisions between various atoms and electrons or hydrogen atoms, are needed for a proper modeling of atomic and molecular excitation as well as spectral line radiation, but these data are often missing. If both these assumptions are to be relaxed simultaneously, the radiative transfer in 3D will be very computer demanding, and considerable approximations will be needed in calculating the radiative energy transport. The replacements of the assumptions of LTE and MLT, viz. statistical equilibrium and hydrodynamics, are also physical approximations in themselves, though most probably valid for photospheres (but not for the outermost thinner atmospheres). More problematic for the modeling of photospheres and their spectra may be the neglect of magnetic fields and the simplified lower boundary condition of the models. In more realistic models the dynamics like pulsations or waves, and the magnetic fields of these boundary layers resulting from deeper dynamos, may be vital, at least for certain types of stars.

From this helicopter view we shall now proceed closer to inspection of the contemporary detailed modeling of various types of stellar atmospheres. The focus will continue to lie on the formation and interpretation of photospheric spectra, which is the dominating diagnostics of stellar abundances.

4. The solar-type stars

The solar-type stars, by which I here mean main-sequence stars in the spectral interval mid F to late K, including Pop II stars, have for a long period played a key role in the analysis of nucleosynthesis and galactic evolution. For these stars spectral analyses can naturally be carried out differentially relative to the Sun, which means that systematic model errors may be assumed to cancel out to some degree with standard models, if the analysis is made carefully. Nevertheless, this is also the type of late-type stars for which more advanced models beyond the standard 1D LTE MLT recipe have been carried out and applied to abundance analysis (see Asplund, 2005, for a comprehensive review).

A most impressive development is thus the calculation of 3D models where the hydrodynamical equations are solved in spatial grids of \( (\times 100)^3 \), and many time steps, with the radiative transfer treated such that the energy transfer through radiation is described in some detail (see, e.g., Nordlund, Stein & Asplund 2009, Collet, Asplund & Trampedach 2007, Freytag 2008, Ludwig & Kucinskas 2005, Ludwig & Steffen 2008, and references therein). The models are able to reproduce a number of observed properties for the solar and stellar photospheres, such as the appearance and time scales of solar granulation, line profiles with bi-sectors and line shifts for the Sun and the stars and, most recently, centre-to-line variations of solar spectral lines and continua (Koesterke et al., 2008, Pereira, Asplund & Kiselman, 2009) to an astounding accuracy.

An especially interesting result is that the 3D models of the more metal-poor stars deviate much more from standard models in the surface layers (see Asplund 2005 and references therein) than is the case at solar chemical composition. Thus, the mean temperatures for \([\text{Fe/H}]=-3\) models (else solar parameters) in 3D may be about 2000 K cooler in the surface layers than a standard model. Physically, this is due to the convective
motions in the upper layers which lead to expansion cooling. This corresponds to layers above the unstable hydrogen ionization zone in a 1D model, where the standard MLT does not allow convection at all. Although the correct calculation of the radiative energy transfer in these upper layers of the 3D models may still be a problem (only a relatively small number of frequency points can be afforded), the results seem to suggest that very considerable adjustments of standard abundances for such stars have to be made. For elements based on spectral lines from molecules (like CH, NH and OH) these abundance corrections downwards may amount to more than 1 dex (Asplund & García Pérez 2001, Collet, Asplund and Trampedach 2007, see also Behara et al. 2009, and Hernandez et al. 2008). Even for abundances derived from low-excitation atomic lines, the effects may be very considerable (see Bonifacio, Caffau & Ludwig 2009, who find effects of as much as 0.8 dex in the Cu abundances for Pop II dwarfs).

Very considerable progress has also taken place in the latest decade in the calculation of stellar spectra with the assumption of LTE relaxed, and a great number of different elements have now been studied with detailed statistical-equilibrium calculations in the formation of solar-type stellar spectra, not a least as a function of stellar metallicity (e.g., from the last few years for Li: Shi et al. 2007, Lind et al. 2009; N: Caffau et al. 2009; O: Caffau et al. 2008, Fabbian et al. 2009; Na: Gehren et al. 2004, 2006, Liu et al. 2007, Andrievsky et al. 2007; Mg: Gehren et al. 2004, 2006, Liu et al. 2007, Sundqvist et al. 2008; Al: Gehren et al. 2004, 2006, Liu et al. 2007, Andrievsky et al. 2008; Si: Shi et al. 2008, K: Zhang et al. 2006; Ca: Mashonkina et al. 2007; Sc: Zhang, Gehren & Zhao 2008; Mn: Mergemann & Gehren 2008; Fe: Collet, Asplund & Thévenin, 2005; Co: Bergemann 2008; Sr: Short & Hauschildt 2006; Ba: Short & Hauschildt 2006, Andrievsky et al. 2009; Nd: Mashonkina et al. 2005. For earlier studies, see Asplund 2005). As mentioned above, an important problem in these SE studies is the shortage of accurate cross sections for atomic inelastic collisions with electrons and hydrogen atoms (note, however, the point made by Gehren et al., 2006, that this in not always very problematic). One must in general be critical concerning the classical or semi-classical recipes that are often used for the collision cross sections in the absence of more adequate quantum-mechanical data. Also, the semi-empirical derivation of collision cross sections from solar (or stellar) data, by requiring observed solar line strengths to fit the calculated ones, is risky, since problems with the solar model or model atom may be hidden in this fit, preventing correct cross sections from being derived. However, proper quantum-mecanical calculations are getting possible (current work by Belyaev, Barklem and others) and this seems to be the way to go, with laboratory checks for measurable transitions. An interesting aspect which is also illustrated by the work by the latter authors is the need to care about details in the model atoms of the statistical-equilibrium calculations. Thus, Barklem (2007) found that the correct treatment of the electron-impact excitation of OI from the triplet 3s to the singlet 3s state causes very significant corrections of the oxygen abundances, as derived from the OI IR triplet lines, and Barklem et al. (2003) and Lind et al. (2009) showed that the standard semicalssical collision rates for H+Li collisions are highly exaggerated and tend to lead to underestimated Li abundances for Pop II stars, but also that the charge transfer Li+ + H → Li++H− has even more severe effects in the converse direction on the abundances. In abundance analysis at least, “the devil is in the details”.

Another key factor to worry about is the need for realistic UV fluxes in these calculations, not the least for the proper estimation of photo-ionization rates. Here, the different atomic species cannot always be treated individually; e.g. the departures from LTE for Fe (leading to over-ionization which increases the UV-flux of the model) may couple to the statistical equilibrium of other elements like Sr and Ba (see Short & Hauschildt 2006).
As yet, very few model atmospheres for late-type stars have been calculated with the LTE assumption relaxed. The pioneering NLTE solar models made by Anderson (1989) have now been replaced by those of Short and Hauschild (2005) in which 24 different elements were consistently treated in SE, with up to 6 different ionization stages each, and thousands of individual transitions for each species. The resulting 1D solar model structure is a few hundred K hotter in the surface layers than the corresponding LTE model. Its UV flux is also significantly higher. These effects are to be expected, the first one as a result of the loosening of the radiative transfer from the local temperature (more lines formed in scattering processes) and the over-ionization of primarily iron. For the K giant Arcturus, Short and Hauschildt (2003, 2009) find again a significantly higher UV flux but a conversely cooler SE model as compared with the corresponding LTE model. This latter result is not understood in detail, but one may speculate that it is due to the surface CO cooling, which gets more dominating for the K giants if the metal-line opacity is decoupled from the local gas.

How far have we come in joining the 3D approaches with the statistical equilibrium (SE) treatment of excitation and ionization of the gas and of radiative transfer? Some diagnostic work has been done so far, with calculation of solar and stellar spectra in SE from a 3D model, the latter, however, constructed under the assumption of LTE. This work includes studies of Li by Asplund, Carlsson & Botnen (2003) and O by Asplund et al. (2004), of Na and Ca by Uitenbroek (2006), and, although not with a complete 3D treatment of radiative transfer, of Fe and O by Shchukina, Trujillo Bueno & Asplund (2005) and of Sr by Trujillo Bueno & Shchukina (2007). We also note that Hansteen et al. (2004, 2007) and Leenaarts et al. (2007, 2009) have developed magneto-hydrodynamic models of the upper solar atmosphere with descriptions of the radiative transfer in the most important transitions in considerable detail. The number of atomic levels one can afford in problems of this character is a severe restriction, although Carlsson (2008) has argued that atoms with typically 10^2 levels should presently be possible to handle if the most efficient methods are optimized. The already available results are, however, quite interesting and clearly demonstrate the complexity of the situation. One example is the results for Fe I and Fe II of Shchukina, Trujillo Bueno & Asplund (2005) which indicate that the Fe abundances for a subdwarf \((T_{eff}/\log g/[Fe/H]) = 5700K/3.7/−2.5\) are underestimated if LTE is assumed relative to SE by about 0.5 dex (due to over-ionization) while it is overestimated by 0.3 dex if 1D MLT LTE models instead of 3D hydrodynamical LTE models are used (which essentially is due to the surface expansion cooling in the 3D model). Here, one would expect that the combination with SE+3D would lead to an effect in between, but it turns out instead to be an almost as large positive effect as for the “pure” SE case. A naive adding of the two separate effects would lead to an underestimate of \([Fe/H]\) by about 0.25 dex. Also for Fe II, the two effects combine in a clearly non-linear way.

Fully consistent and realistic hydrodynamic 3D models in SE have still not been constructed, and it is unclear whether such a project can be undertaken with existing algorithms and computers. In taking this on it would be necessary to find an adequate treatment of the radiative transfer, e.g. by reducing the number of atomic levels involved and the points in the frequency spectrum to a small number of representative levels and frequencies, respectively, but still producing a realistic radiative field. Important steps in developing such methods were taken by Nordlund (1982) in developing his “opacity-binning method”, by Skartlien et al. (2000) in including scattering in such treatments, and by Trampedach (unpubl.) in optimizing the choice of frequency points further. It seems, however, that decisive and final steps towards physical consistency, entailing both 3D and SE for photospheres will have to wait for further computer development.
An important question is then what errors in abundances one may expect as a result of this lack of consistency. The gradual development of SE and 3D models in recent decades has along the way generated a number of estimates of systematic errors due to the neglect of each of these complications in standard models. Looking back at such estimates it is fair to say that they were often off, sometimes severely exaggerated, but not seldom also severely underestimated. This certainly reflects the complexity of the phenomena. While in the standard radiative-equilibrium model atmosphere (most MLT models are also in radiative equilibrium in the upper layers) the local temperature is simply set by the balance between heating by absorption of radiation from the deeper atmospheric layers, and cooling by emission from the local gas, in the hydrodynamic case the compression and expansion heating/cooling are also decisive. These dynamical effects affect the capacity of the gas to absorb and emit radiation. So, the coupling between hydrodynamics and radiation gets very intricate. With all this in mind, I would still dare to conjecture that the abundance errors caused by the neglect of coupling SE and 3D hydrodynamics in the models may well amount to 0.1 dex for numerous chemical elements in solar-type stars.

5. M stars, cool super-giant stars and AGB stars

For the M stars, the dominance of opacity sources like TiO and H$_2$O introduces further complications but also some simplification, since the significance of the very numerous metal lines gets smaller. Note, however, the importance of getting the ionization equilibria of the electron contributing elements (Mg, Al, Ca, Na, and K) right, since they contribute electrons to the still strong continuous $H^{-}$ opacity as well as opacities from other negative ions. Also, the ionization of Ti, as well as of La, Zr and V, is important to describe correctly, since the number of neutral atoms is directly determining the number of oxide molecules. While the opacity data of TiO, as well as of water, have improved considerably in the last decades, one may still worry that the numerous electronic transitions of TiO may be out of LTE. In LTE, these transitions considerably heat the upper layers of the M star models. If the lines are formed in more scattering-like processes this heating is expected to be much reduced. For the cooler M stars and in particular for the C stars the opacities of the polyatomic molecules are still not satisfactorily known for many species. An even more severe problem for these stars is the dust opacity; in practice, the dust composition, size distribution and optical properties have to be parametrized with several uncertain parameters. A particularly interesting problem, which will not be further discussed here, is the modeling of atmospheres of the coolest M stars and the brown dwarfs (see Chabrier, Baraffe, Allard & Hauschildt 2005 for a review).

Ludwig, Allard & Hauschild (2002, 2006) have calculated a number of model 3D hydrodynamic models atmospheres for M stars of different gravities and temperatures and compared with corresponding 1D models. The authors find smaller temperature contrasts for the convection inhomogeneities of these stars than for the solar-type giants, which was to be expected in view of their smaller fluxes. However, they also demonstrate, for solar metallicities, that the models can be well fitted by MLT models. For this to be useful in practice, however, one must know beforehand, e.g. from 3D simulations, what value of the mixing-length parameter ($\alpha = l/H_p$) to use. Also, as demonstrated by the authors, the near IR flux formed in the upper layers of the atmospheres is severely dependent of the temperatures in these layers and show significant differences between the 1D and 3D models. In a recent paper, Kucinskas et al. (2009) compared abundances derived from a 3D model of an M giant atmosphere with those of a corresponding 1D model. They found small differences for abundances derived from lines of neutral atoms and molecules, but rather considerable differences if ionic lines were used.
An interesting result from the 3D simulations is that the surface granulation pattern in general looks very similar for a very wide range of stellar surface gravity (Freytag & Ludwig, 2007). The characteristic size of convection elements, or granulae, scales as $H_p$, which means (as was already predicted by Schwarzschild, 1975) that the surface of the super-giant stars will be covered with a few giant convection elements, although finer structures may also occur. All this is clearly seen in the 3D hydrodynamic “star-in-a-box simulations” by Freytag (2003). These impressive simulations show a good agreement with the interferometric observations of Chiavassa et al. (2009, see also Kervella et al. 2009) but the radiative transfer in them, basically assuming gray opacities and a coarse grid of points in the atmosphere, is still not treated in the detail needed for high-quality abundance work.

For atmospheres of supergiants and AGB stars, the lower boundary condition of the model atmosphere is obviously crucial for the whole model structure. These stars of almost always pulsating, more or less regularly. For several decades, such atmospheres have been modeled by 1D dynamic models, set in pulsation by a lower piston. Here, the piston amplitude and frequency are free parameters. Such models were pioneered by Wood (1979) and Bowen (1988) and later developed by Fleischer, Gauger and Sedlmayr (1992), Höfner & Dorfi (1997) and subsequently by the groups in Berlin, Vienna and Uppsala. The models also have a free outer boundary condition, and a basic aim is to study stellar mass-loss: the gas is elevated and expanded by the pulsations, such that dust can form and, driven by radiative forces, drag the gas along. More recently, the models have included non-gray opacities (Gautschy-Loidl et al. 2004), dust formation with a two-phase treatment of gas and dust (Sandin & Höfner 2004, and references therein, Sandin 2008), and extensive grids of models have been calculated (Mattsson et al. 2009).

Freytag & Höfner (2008) have recently added possibilities for dust to form in a 3D simulation for a carbon AGB star by Freytag’s program. Indeed, plumes of dusty gas are expelled from the model (similar to those later found by Kervella et al. 2009 for Betelgeuse), and when following the dust development further out (using a 1D hydrodynamics code) the authors find final wind velocities characteristic of carbon stars and in fair agreement with 1D models.

Finally, it should be noted that the effects of magnetic fields on super-giant atmospheres were explored by MHD “star-in-box” simulations by Dorch (2004). He found that “local dynamos” driven by the giant convection motions generated considerable large-scale magnetic fields of up to 500 Gauss and that this field at the densities characteristic of the tenuous photospheres of these stars could have considerable effects on their structures.

It is still premature to give figures on how these various improvements, and uncertainties, in the modeling of M and C stars will affect the abundances derived from their photospheric spectra. No doubt, the progress basically demonstrated for the solar-type stars as regards convection and departures from LTE will apply also in this case, although as regards the statistical-equilibrium calculations the demands for physical data are different since molecular transitions are more at focus. Also, at least for the super-giants, the convective dynamics will be more violent and partly supersonic. As compared with the solar-type stars, in a sense more “elementary” demands (complete opacities) and more “advanced” physics (dynamic lower boundary conditions, dust formation, magnetic fields) are also important. Another aggravating circumstance in the cool-star case is that there is no nearby star like the Sun to compare the models directly with. Previous studies of uncertainties from standard models tend to suggest abundance errors ranging from 0.15 - 0.40 dex for M and C stars. Since the coupling between the various unknown properties of the phenomena at play is so intricate, it would not be very astonishing if
errors of this order of magnitude will still remain after the implementation of 3D models, and with state-of-the-art consideration of dust opacities, lower-boundary conditions and magnetic fields. However, if so, the error estimates will be much more well-founded.

6. What does all this mean for abundances?

Indeed, the progress in modeling stellar atmospheres in the last two decades has been impressive! However, recent advanced models may still not be ready for large-scale applications, just because they have not been calculated or carefully tested for very many sets of stellar parameters, or because they still lack important details in order to be reasonably realistic. What should the poor observer, wishing to deduce reliable abundances, do when models are improving in complexity and in detail but are still not available for the stars observed, and the systematic error estimates seem to get better motivated by still remain considerable? Here is some simple advice:

1. Be anxious to observe abundance criteria of different type, when possible (different excitation, ionization, atomic and molecular, etc), and inter-compare! This will give more reliable abundances including error estimates, as well as possible clues towards inadequacies in the models.

2. Give highest weight to abundance criteria that are not very temperature sensitive! In addition to reducing the uncertainties caused by the uncertain effective-temperature scale, this also reduces the errors due to thermal convective inhomogeneities.

3. Try to rely more on “majority species”, i.e. dominating species of ions or molecules (e.g. Fe II and not Fe I for F and early G stars, CO for determining C abundances for K stars sooner than C\textsubscript{2}, etc), since their number densities are less affected by departures from LTE and uncertainties in temperature! There may be modifications to this rule when the stellar gravities are not very well known (e.g., a minority species like Fe I for F-G stars scales with electron pressure like H\textsuperscript{+} which thus compensates for the gravity uncertainty).

4. Do not rely heavily on saturated spectral lines, whose strength is determined by velocity fields and stellar surface temperature more than by abundance! Instead, prioritize the observing programmes such that weak lines and wings of strong lines may be adequately measured.

5. Make careful differential analyses, by comparing stars with very similar fundamental parameters such that one expects the systematic model errors to cancel! Examples of the progress that may achieved in this way are given by Meléndez et al. (2009 and Meléndez’s talk at this Symposium).

6. Check abundance determinations for cool stars by comparison with solar-type stars with presumably the same (initial) chemical composition from binaries or clusters! Although this method must be used with caution, due to dredge-up of processed material in evolved stars, and the effects of diffusion at earlier stages (cf. Korn et al. 2006), it should be systematically advanced across the HR diagram.

7. Support the few groups doing advanced 3D and SE modeling of late-type stars, and not the least those producing the physical data needed! This plea is for scientifically collegial and moral support, but frankly speaking also for economical support. Since a considerable number of the authors of the 4000 annual papers with abundance in the Abstract are likely to sit in committees of financing bodies I propose a simple calculation: a typical cost for one of these papers can be estimated to be at least $10^4 US$. For a few percent of the total cost of these papers, the number of positions for advanced stellar-atmosphere modelers and physicists supplying data could be doubled. Would it not be worth it?
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