A New Freely-Downloadable Hands-on Density-Functional Theory Workbook Using a Freely-Downloadable Version of deMon2k

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Abstract

One of us (MEC) developed a hands-on workbook for density-functional theory (DFT) during the summer of 2020. The idea was to have something that could be used to provide practical teaching for students at the Masters or advanced undergraduate level that would be free, could be used on a student’s own personal computer, and would complement formal course work. The workbook is also very much intended to encourage students to explore program options, discover theory limitations, puzzle out what to do when the program does not work as expected, and to help students transition to thinking and using quantum chemistry programs as a researcher might do. After describing the structure of the workbook, we describe how the workbook has been used thus far as a teaching tool and as a useful step towards research-level problems.

1 Introduction

“I hear and I forget.
I see and I remember.
I do and I learn.”
— A popular proverb frequently attributed to Confuscious

“Quantum chemistry” generally refers to the fine art of calculating the various properties of molecules by solving the Schrödinger equation. It normally involves running programs of various
degrees of complexity. Within quantum chemistry, terms like "theoretical chemistry" and "computational chemistry" nowadays sometimes seem to be used interchangeably. However there is at least a historical difference between the theory behind the programs that quantum chemists use and a computational chemistry course intended to teach users (whose main interest may be experimental synthetic or physical chemistry) how to do routine calculations with routine programs. This difference is also reflected in different textbooks which are used to teach these subdisciplines. For example, a typical trajectory for an advanced physical chemistry student interested in deepening their knowledge of quantum chemistry might be to learn some basic quantum mechanics from a good third year undergraduate physical chemistry book such as McQuarrie and Simon [1], then use Levine’s excellent text [2] in a fourth-year course, followed by Szabo and Ostland [3] in a first graduate school course, possibly followed by Helgaker, Jørgensen, and Olsen [4] in an advanced theory course. Computational chemistry could be introduced beginning as early as the students third year of undergraduate studies and might use Cramer’s book [5] or Jensen’s book [6], to name just two possibilities. However something seems to be missing that is often supplied only partly by tutorials for specific programs. Specifically, the problem with the tutorials is that they typically show how to do calculations without actually having students explore program options, discovering theory limitations, and puzzling out what to do when the program does not work as expected. Students need this to transition to thinking and using quantum chemistry programs as a researcher might do. This is why one of us (MEC) spent time in the summer of 2020 developing a freely downloadable workbook [7] which will just be referred to here as the Workbook (with a capital W). It uses a freely downloadable LINUX serial version of the DEMON2K program [8]. This means that the student can download a fully functional quantum chemistry program onto their personal computer for free and run it there to gain valuable experience about how such a program works. This is not intended to replace existent courses and basic textbooks, nor do we feel that the applications in the Workbook are particularly specific to DEMON2K. (We are not trying to claim that our software is better than other software for present purposes.) Rather we propose this Workbook as a valuable (but freely available) complement to existing resources. The goal of the present article is to describe our pedagogical experiences with this Workbook thus far and where we hope to go in the future. As we will frequently need to refer to specific authors, we will do so by their initials only. For example, MEC is one of the authors of DEMON2K and so it was very natural for him to base the Workbook on this program.

This article is organized as follows. The next section says a few words about DEMON2K and about the organization of the Workbook. The Workbook has been β tested by NBO and AP, two students at very different levels. Section 3 focuses on NBO, an advanced (i.e., third-year undergraduate) β-tester of the Workbook. It does not seem necessary to document the experience of AP who had fewer obstacles to surmount in using the Workbook. However, Sec. 4 reports how the Workbook unexpectedly opened up an avenue for research in Cameroon in Africa, where computational resources are significantly more limited than in France, specifically in the context of the PhD thesis work proposed by AJE for her thesis student AP. Section 5 sums up our principle conclusions and hopes for the future.

2 Workbook 1

The Workbook was designed with first-year Masters students in mind who have already had some introduction to quantum chemistry, perhaps following the cursus already mentioned in the introduction. The Workbook is intended to be complementary to this and to further instruction in quantum chemistry and density-functional theory (DFT) in particular. Those who are seeking more information about DFT may be referred to a number of useful basic texts [9, 10, 11]. The reader may also
be interested in a recent perspective article discussing the place of DFT in present-day quantum chemistry \[12\]. The goal here is not to review either basic quantum chemistry or DFT more than necessary. Rather we just seek to provide an overview of the Workbook. This is most conveniently done by structuring the subsections of this section in the same way as the structure of the Workbook.

2.1 Preliminaries

The first part of this chapter is just a

Preface explaining the objectives of the Workbook. One of these objectives was to help train students new to DFT in quantum chemistry, such as NBO and AP. This is then followed by an important part called

Installation which describes how to download and install a serial version of the \texttt{deMon2k} program \[13\,8\] from the \texttt{deMon2k} website. This version should run on any Linux machine, including personal computers, making it highly convenient for self-study and teaching purposes. Of course, many people do not have Linux installed on their personal computer, but this can be circumvented by installing first \texttt{VirtualBox} and then the Ubuntu version of Linux as NBO explains in an appendix to the Workbook. A final part of this chapter is

Lesson 0: Running the Program This involves setting up a simple C shell program \texttt{run.csh} which takes care of the administration of the various files created and used by \texttt{deMon2k} by using a simple command such as \texttt{run.csh 02} which takes information from the file \texttt{02.inp} and runs \texttt{deMon2k}. The program \texttt{run.csh} is deliberately kept simple in order to encourage the student to understand and modify it as appropriate.

2.2 Hydrogen Atom Calculations: Basis Sets and Functionals

The first part is

Lesson 1: The Orbital Basis Set which is aimed at familiarizing the student with the concept of the linear combination of atomic orbitals (LCAO) approximation,

\[
\psi_i^\sigma(\vec{r}) = \sum_{\mu} \chi_{\mu}(\vec{r}) C_{\mu,i}^\sigma. \tag{1}
\]

Here \(\psi_i^\sigma\) is the \(i\)th molecular orbital (MO) of spin \(\sigma\), \(\chi_{\mu}\) is an “atomic orbital” (AO), and \(C_{\mu,i}^\sigma\) is the corresponding matrix of MO coefficients. In practice, the AOs are no longer solutions of an atomic Schrödinger equation but rather are atom-centered functions chosen for computational convenience as well as for their ability to cover the variational space. The most common choice in quantum chemical programs is to use gaussian-type orbitals (GTOs) as most of the integrals may be evaluated analytically. We note in passing that \texttt{deMon2k} (or, more exactly, \texttt{deMon} for \textit{densité de Montréal}, before it was renamed) was one of the first programs to use GTOs for DFT and hence to be able to take advantage of the large amount of quantum chemistry technology available at that time for calculations using GTO basis sets. Optimization of the MO coefficients uses the variational principle. Hence this is not only a lesson about GTO basis sets, but about the proper use of the variational principle when comparing results from different basis sets.

This is followed by
Lesson 2: Density Functionals  which introduces the numerous density-functional approximations (DFAs) which are available in deMon2k (and in many other quantum chemistry programs as well). Some exact conditions are discussed, notably the self-interaction error, and an exercise is proposed to test the quality of the different DFAs for the total and orbital energies of the hydrogen atom where the exact answer is known.

2.3  $H_2^+$ and $H_2$: Functionals, Potential Energy Curves, and Geometry Optimizations

The student finally gets to molecules, albeit the simplest possible molecules. This chapter of the Workbook begins with

Lesson 3: The Radical Dissociation Problem  in which the notorious dissociation problem of $H_2^+$ is discussed in terms of the particle-number derivative discontinuity present in the exact exchange-correlation functional, but absent in nearly all DFAs (with Hartree-Fock an exception, to the extent that Hartree-Fock may be considered to be a DFA). As is the case with all of the lessons, exercises are proposed to help the student obtain a practical understanding of the non-trivial concept that has been introduced. Answers to all the lessons are given in the last chapter of the Workbook. The student is likely to encounter their first real difficulty in this lesson — namely the need to modify the sample input file when using meta generalized gradient approximations. The needed modification is explained in the answers in the final chapter and a lengthy discussion is given analyzing and discussing the results.

The next lesson is

Lesson 4: Treating Multideterminantal Problems by Symmetry-Breaking . This is an application to $H_2$ where DFAs work reasonably well, provided the trick of symmetry breaking is used. It is also an excuse to discuss spin coupling and dissociation limits. Symmetry breaking and spin projection is introduced. The exercise is more challenging because DFT calculations do not necessarily automatically converge to symmetry-broken solutions unless the user is creative in how the program is run. The problem of self-consistent field (SCF) convergence is also typically particularly severe near symmetry-breaking points. This is a good chance for students to explore the different tricks for making their calculations converge.

The final lesson in this chapter is

Lesson 5: Analytic Gradients and Geometry Optimization . Variational calculus is introduced as a formal tool and then used to derive the Hellmann-Feynman theorem which fails for atom-centered GTO basis sets. It is then explained why Pulay forces need to be introduced and why, in practice, these require good SCF convergence. A simple potential energy surface walking algorithm is introduced and discussed. The exercises show that the walking algorithms used in deMon2k are actually much better than the simple algorithm that was proposed.

2.4 Lesson 6: Singlet Oxygen, $^1O_2$

This chapter is a bit unusual because it was intended as a lesson on the multiplet sum method to help AP get started with his PhD thesis project involving reactive oxygen species. It is a nice lesson in group theory applied to multideterminantal wave functions. This lesson would grow into a research
paper [14] comparing how well different functionals describe the ground and lowest excited states of diatomic oxygen as further described in Sec. [4].

2.5 Answers

This contains answers to the exercises proposed in the various lessons as well as in-depth analysis and discussion. It is hoped that the student will only look at this after trying the exercises on their own. It is possible that the student will find better solutions to difficulties encountered than the ones given in this chapter.

2.6 Installing Linux on a Mac Notebook

This appendix, written by NBO, describes how she was able to install Linux on her Mac Notebook by first installing VirtualBox and then installing Ubuntu.

3 Advanced Undergraduate Experience

Early in 2022, NBO volunteered to β test the Workbook as part of a one-month research internship as a third-year undergraduate in chemical physics. Her experience is summarized in her report (in French) which may be found on-line [15]. In the jargon of computer programming, α testing refers to debugging (and other tests) performed by the programmers, while β testing refers to additional testing made by users which may turn up new errors or just show where further program development is useful to meet their needs. Similarly we can say that both AP and NBO were β testers for the Workbook. However NBO was testing it as someone very new to quantum chemistry — namely as an undergraduate who was just taking her first quantum physics course at the same time as her one-month research internship. We were very curious to see if she could benefit from the Workbook. Given that her background at that time was about the minimum needed, we focused on Lessons 0 and 1.

Lesson 0 was to see if she could install and run demon2k on her Mac notebook. She passed this first hurdle with flying colors and contributed a key appendix on the subject to the Workbook as described in Sec. [2].

Here we focus on her work with Lesson 1. This Lesson was considerably simplified by focusing only on the problem of constructing GTO basis sets for solving the hydrogen atom as exactly as possible and comparing against the known exact solutions. In order to be able to treat this one-electron system as exactly as possible, NBO carried out self-interaction error free Hartree-Fock calculations using the FOCK option. NBO was then free to focus on the details of GTO basis sets and on the variational principle. For reasons of simplicity, Hartree atomic units ($\hbar = e = m_e = 1$) will be used throughout this section.

She began with the classic textbook exercise of finding the variationally optimal exponent of a single GTO,

$$\psi_{\text{trial}}(\vec{r}) = \left(\frac{2\alpha}{\pi}\right)^{3/4} e^{-\alpha r^2}.$$  \hspace{1cm} (2)

The radial hamiltonian is,

$$\hat{h} = -\frac{1}{2r} \frac{\partial^2}{\partial r^2} r - \frac{1}{r} + \frac{1}{2r} \hat{L}^2,$$  \hspace{1cm} (3)
where $\hat{L}$ is the angular momentum operator which acts as an annihilation operator on the $s$-type function $\psi_{\text{trial}}$. From this, it is then a straightforward exercise (involving gaussian integrals which, by coincidence, NBO was also studying in her quantum physics class at about the same time) to determine that the variational integral is 

$$W(\alpha) = \frac{3}{2} \alpha - 2\sqrt{\frac{2\alpha}{\pi}}.$$  

(4)

Taking derivatives and setting equal to zero leads to analytic expressions for the variationally optimal value of $\alpha$ and the associated energy:

$$\alpha_{\text{min}} = \left(\frac{2}{3}\right)^2 2\pi = 0.2829$$

$$E_{\text{min}} = W(\alpha_{\text{min}}) = -0.4244.$$  

(5)

It was very important for NBO to be able to verify this explicitly by creating her own single function GTO in the deMon2K BASIS file where she could modify the exponent $\alpha$. This resulted in the graph shown in Fig. 1 which comforted NBO by showing that the program gave the same results as she had found. This, of course, occurs because of the use of explicit formulae for gaussian integrals within the deMon2K program.

The next step was to go beyond the sort of exercise normally found in textbooks to something looking more like research. The “research question” was,

How can a GTO basis be constructed that systematically converges to the exact answer and how large does it have to be for a given level of accuracy?

To this end, NBO constructed a series of even-tempered basis sets [16, 17, 18], meaning that the GTOs that she put in the BASIS file were sets of $s$-type GTOs of the form of Eq. (2) but with a

The series of $\alpha_i = \alpha_0 \beta^{i-1}$ for integer $i$. Even-tempered basis sets are known to optimally cover variational space in a certain sense, making them a good choice. She chose $\alpha_0 = 0.00221015625$ and $\beta = 2$ with $i = 1, 2, 3, \ldots, 19$, so that $\alpha_8 = \alpha_{\text{min}}$ of Eq. (5) obtained by her hand calculation plus added tight and diffuse functions. Results are shown in Fig. 2. Part (a) of the figure shows that the energy decreases significantly when NBO added more and more tight functions (A-D) and also when she added a first more diffuse function (E), but not when she continued to add more diffuse functions (F-K). After that NBO added more ands more tight functions (J-S) until agreement with the exact energy was nearly $10^{-6}$ Ha = 0.0006 kcal/mol. Part (b) of the figure shows that the wave function is also converging, with an improved description of the long range and especially of the cusp behavior. Part (c) of the figure tests a consequence of what physicists call the Hylleraas-Undheim-MacDonald theorem and what mathematicians call Cayley’s interleaving theorem which says that adding additional basis functions in a linear variational problem can only result in a new set of eigenvalues that interleave the old eigenvalues. In the present context, this means that every $n$th energy is an upper bound to the true $n$th energy level. In contrast to the ground-state situation, and as expected, we see that adding diffuse functions is essential for proper convergence of excited-state energies.

The above description of what NBO did is not an exhaustive list of everything done during her short, but very productive, one-month internship. What is more important is that she was able to do quite a lot, in no small part, because of the availability of the Workbook as a learning tool and because she could work directly with her own personal computer. She even went beyond what was described in the Workbook to make her own exercises. We believe this is very much in the spirit of the Workbook which aims at providing tools, and the learning environment needed, for self-learning and moving towards research using quantum chemistry. But let us translate NBO’s own conclusions directly from her internship report:

“The advantage of the software used and of the Workbook is that a student can learn and progress by themselves in learning DFT armed with only their computer. For this reason, I can recommend the Workbook to other students interested in a hands-on approach to basic quantum chemistry.”

4 Gateway towards Research

This section describes how the Workbook became a gateway towards research-level work performed on computers in Cameroon and published in a peer-reviewed research journal [14]. This is significant because of the high-level of interest in theoretical research in Africa, but a real lack of computational resources combined with an, at least partially incorrect, perception that such resources are needed to do cutting edge research. AJE and MEC are happy to acknowledge the African School on Electronic Structure Methods and Applications (ASESMA), with which we have been involved since 2012, for helping to create a research environment in Africa where efforts such as our own are possible.

We are also happy to learn that Jim Gubernatis will receive the 2023 John Wheatley Award of the American Physical Society, “For ongoing commitment to developing physics in Africa through initiating the African School on Electronic Structure Methods and Applications and leadership in bringing together African physicists from across the continent to create a Pan-African physics communication vehicle.” ASESMA was established to improve the research environment for Africans doing theoretical research in Materials Science and had its first meeting in 2008 [19-23]. Quantum chemistry has been a part of ASESMA from very early in the history of the school. In fact, theoretical solid-state physics and quantum chemistry have enormous overlaps, even if their language and approximations differ. This difference has been diminishing over the years as solid-state
Figure 2: Results of NBO’s numerical experiments with the even-tempered basis sets that she constructed herself: (a) groundstate energy error \( p\Delta E = -\log_{10}(E - E_{\text{exact}}) \) for the different basis sets, (b) convergence of the wave function, and (c) convergence of excited state energies (X stands for “exact”).
physics focuses more on nanostructures and as quantum chemists turn towards ever larger systems. Partly for this reason, and partly because of the lack of anything analogous to ASESMA for quantum chemists in Africa, there has always been a subgroup of ASESMA theoreticians interested in quantum chemistry.

ASESMA students and African mentors still have to face substantial problems. A bottleneck in Africa has been scarce computing resources as many African countries, such as Cameroon, provide little governmental support for research. This is partly made up by access to computing resources via collaborations with researchers in developed countries and partly by limited access to high-performance computing centers in wealthier African countries, notably South Africa. But, we feel that this does not replace the need for local computational resources for education and for research which should not always require large amounts of computational resources. This is one place that the Workbook can be very helpful as it is based upon freely downloadable software that will run on any Linux system. AJE and AP already had some experience with solid-state quantum physics codes which typically use very different types of basis sets than do quantum chemistry codes. As the thesis subject proposed by AJE for AP focuses on molecules in a biological context, AP needed to be trained in different methods. This was one of the reasons (but not the only one!) that MEC developed the Workbook in the first place. It has been used by AJE and MEC to help train AP and the Workbook is actually subtitled “Abraham’s Workbook” as he was the first β tester.

Rather than describe AP’s β testing experience (which was positive), we focus instead on how the Workbook became, almost accidently, a gateway to computational work that could be carried out locally using only the limited computational resources available locally in Cameroon and published in an archival research journal [14].

The research project proposed by AJE as AP’s thesis project concerns the use of buckminsterfullerene (C₆₀) and its derivatives as antioxidants that may be used to protect the body and the environment from highly reactive oxygen species (ROSs). These later include a variety of small molecules. Although ground-state $^{3}\text{O}_2$ (which is in a triplet electronic state) is a notoriously benign biradical, for kinetic reasons, it can easily form the highly-reactive superoxide $\cdot\text{O}_2^-$ by reduction or the equally highly-reactive (biradical) singlet oxygen $^{1}\text{O}_2$ by exposure to sunlight in the presence of a suitable photosynthesizer. Other ROSs include, but are not limited to, hydrogen peroxide $\text{H}_2\text{O}_2$ and the hydroxyl radical $\cdot\text{OH}$. ROSs play a role in atmospheric chemistry, water purification, and occur naturally in biology during photosynthesis and during respiration in mitochondria. Needless to say, living things have mechanisms to keep ROSs from getting out of hand, but sometimes extra help is needed. Buckminsterfullerene is so reactive towards radicals that it has been called a “radical sponge” [24] and has even been commercialized under this name for use in cosmetics [25].

The idea then, was to investigate theoretically the reactivity of C₆₀ with ROSs. This led naturally to a discussion of the low-lying excited states of $\text{O}_2$ and inspired Lesson 6 of the Workbook which explains how group theory and the multiplet sum method can be applied to determine the ground- and excited-state energies of $\text{O}_2$. Thus Lesson 6 was designed in the first instance to aid a student to understand a particular approach to a problem.

What happened next was a combination of things, one of which was the very unexpected realization that much of the information on the internet and even in many research articles gives an incorrect, or at least misleading, description of the ground- and electronic-excited states of $\text{O}_2$. It was as if the lessons of Herzberg had been forgotten only a few generations latter! This can explain, at least in part, why only a very few DFT calculations have been done which properly treat the symmetry of $\text{O}_2$ electronic states. It was clearly time to remind the world again of a little group theory (that was in Lesson 6) and to test out which are the best functionals for treating the $\text{O}_2$ multiplet problem (a research-level problem do-able with limited computer resources). This is not
Figure 3: MO diagrams and multiconfigurational nature of the ground triplet state and two lowest singlet excited states of O$_2$. These schematic diagrams are taken directly from the Workbook.

the place to repeat this work, but rather to just review what seem to be the important points.

First of all, the Workbook lessons are presented as a combination of teaching and of self-exploration. For those of us who have been involved in ASESMA, this is an echo of the organization where the first week is devoted to learning concepts and tools while the second week is devoted to a miniproject which might or might not lead to a publication. Lesson 6 was not intended to lead to a publication but the exercises do have the form of a miniproject. Figure 3 shows MO diagrams for the ground- and two lowest excited-states of O$_2$ using real orbitals. The symmetry-imposed configuration mixing is also shown in a schematic fashion. This and a program such as deMon2k which allows MO occupation numbers to be fixed are enough to be able to calculate the energies of all the 3 states from single-determinantal states made from some reference state which we took to be a state having an equal fractional occupation number of half of each spin in each of the two $\pi^*_x$ and $\pi^*_y$ orbitals. Most quantum chemistry programs have some option which allows the creation of this type of reference state, but not every quantum chemistry program allows the changing of MO occupation numbers. It is then a “simple matter” to calculate the three state energies,

$$E[X^3\Sigma_g^+] = E(\pi^*_x[\uparrow], \downarrow[\uparrow], \downarrow[\uparrow]),$$

$$E[a^1\Delta_g] = E(\pi^*_x[\uparrow], \downarrow[\uparrow], \downarrow[\uparrow]) + 2P,$$

$$E[b^1\Sigma_g^+] = E(\pi^*_x[\uparrow], \downarrow[\uparrow], \downarrow[\uparrow]) + 2F,$$

where

$$F = E(\pi^*_x[\uparrow], \downarrow[\uparrow], \downarrow[\uparrow]) - E(\pi^*_x[\uparrow], \downarrow[\uparrow], \downarrow[\uparrow])$$

is the spin-flip energy and

$$P = E(\pi^*_x[\uparrow], \downarrow[\uparrow], \downarrow[\uparrow]) - E(\pi^*_x[\uparrow], \downarrow[\uparrow], \downarrow[\uparrow])$$
is the spin-pairing energy. Previous work on octahedral Fe(II) spin-crossover complexes had shown that the spin-pairing energy ($\tilde{P} = P - F$) can be very sensitive to the choice of density-functional approximation (DFA) \[26, 27, 28, 29, 30, 31\], suggesting that the difference of the $^1\Sigma_g^-$ and $^1\Delta_g$ energies was going to be very sensitive to choice of DFA, but might be better approximated by the use of the OLYP \[32, 33\] generalized gradient approximation (GGA) than by the use of other GGAs.

As no general study of DFAs for $^1\Sigma$ energies had yet been carried out, this was an excellent opportunity to contribute new knowledge to the chemical literature \[14\]. Figure 13 of Ref. \[14\] did indeed confirm that the OLYP error in $\tilde{P}$ was among the lowest of the various GGAs tried. More importantly Fig. 12 of Ref. \[14\] shows that the $^1\Delta_g$ excitation energy is less sensitive to the choice of DFA than is the $^1\Sigma_g^-$ excitation energy, meaning that spin-flip energies are easier to describe in DFT than are spin-pairing energies, at least in this application. We were thus able to contribute something to the knowledge of how different DFAs are able to treat spin. In the end, we found that we had to go fairly high up the Jacob’s ladder \[34, 35\] of DFAs to at least meta-GGAs or even hybrid meta-GGAs in order to get the best level of accuracy \[14\]. Although our paper was only published a year ago, it has already received several citations, meaning that we can make an impact with the Workbook, a freely downloadable serial version of deMon2k, and the level of computational resources available locally in Cameroon.

## 5 Conclusion

A freely-downloadable hands-on density-functional theory Workbook that works with a freely-downloadable serial version of deMon2k, executable on any Linux operating system, has been described. This is a learning tool for serious researchers at the level of beginning Masters students in chemistry or beyond, though we have described the successful use of the Workbook by a third year undergraduate student. It is particularly useful for those who wish to learn at home or who have limited access to computing resources. A specific objective is to create an opening towards research in quantum chemistry precisely by *not* avoiding practical and formal difficulties, but rather by encouraging and helping the student to come to terms with these difficulties.

We think that this Workbook may be especially valuable in the developing world and give an example from Cameroon. Governments in developing countries frequently have little or no funds for scientific research except possibly for the most basic sort of applied research such as water purity analysis. However researchers in these countries are often hungry to do more basic research, but may feel discouraged because of their limited resources. This Workbook is also a wake-up call to those researchers that it is possible to advance science with only limited resources *provided* (and this is the key point) they have enough knowledge to know what are the important fundamental problems and how to contribute to solving them. We would like to think that the Workbook is part of what is needed to enable researchers in both developing and developed countries to educate themselves and find where they can contribute to the advancement of science. We have given one example, but we hope that there will be many others in the coming years.

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Author Contributions

Author credit has been assigned using the CRedit contributor roles taxonomy system [36].

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