



PATENTS ACT 1977

APPLICANT International Business Machines Corporation

ISSUE Whether patent application GB 2117330.7 is
excluded under section 1(2)

HEARING OFFICER Sally Vinall

DECISION

Background

- 1 Patent application GB 2117330.7 ("the application") entitled "Iterative state detection for molecular dynamics data" was filed on 1 December 2021, with an earliest declared priority date of 18 December 2020 in the name of International Business Machines Corporation. It was published as GB 2603607 A on 10 August 2022.
- 2 The examiner issued a combined search and examination report on 20 May 2022. Following four rounds of correspondence between the examiner and the applicant's attorneys, and amendment of the claims, the examiner remains of the view that the claimed invention is excluded as a computer program under section 1(2).
- 3 With the position unresolved the examiner has forwarded the application for a decision by a Hearing Officer based on the papers. The issue of excluded matter before me was set out in the examiner's pre-hearing report of 24 June 2024. The applicant's most recent arguments and the claims under consideration are those filed on 7th March 2024 by the applicant's representatives at Elkington and Fife. I confirm that I have considered all papers currently on file in reaching my decision.

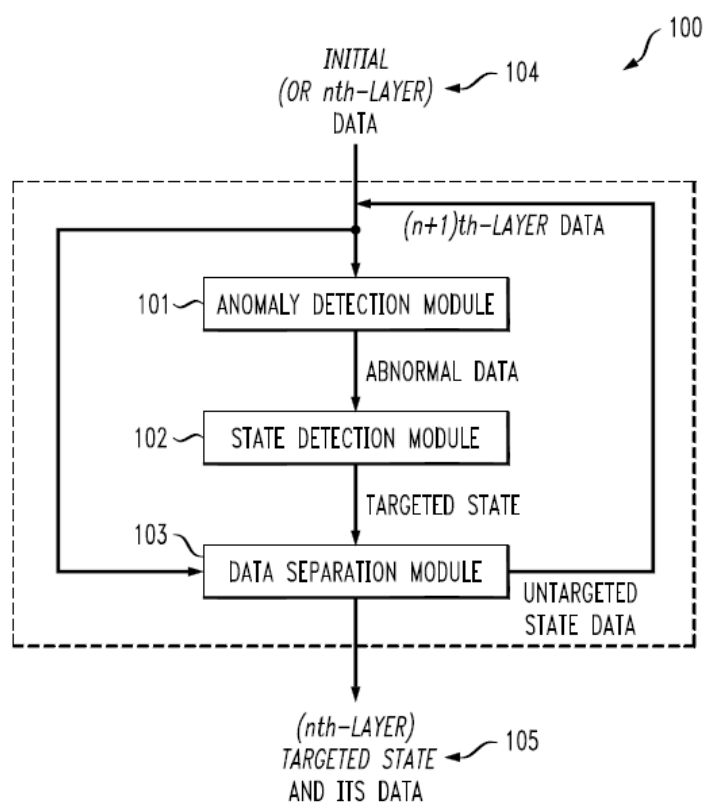
The invention

- 4 The application relates to methods of analysing large data sets and more particularly to a method of identifying unknown molecular dynamic physical states and corresponding samples. Large-scale molecular dynamic simulations generate millions of frames of data, which precludes manual analysis.
- 5 Molecular Dynamics describes a class of computer simulation methods for analysing the physical movements of particles such as atoms or molecules. Molecular dynamic simulations are a tool for the exploration of, for example, the conformational energy landscape accessible to molecules or other particles, interactions between different molecules or particles, etc. The invention is directed to an iterative method of finding unknown molecular dynamic state structures and corresponding samples (e.g., data

points corresponding to a particle/atom or group of particles/atoms). The invention identifies statistically meaningful states in the data, which may be rare. Investigating unknown state structures identified by molecular dynamic data (trajectories/frames) analysis can lead to the identification of, for example, new drug targets.

- 6 Referring to Figure 1 below, a system 100 configured to perform an iterative method of finding unknown molecular dynamic states and corresponding samples according to the invention comprises an anomaly detection module (ADM) 101 separating abnormal data from the total (n th layer) data 104. The layers of data are defined for the iterative method. More particularly, each layer is a defined set of the molecular dynamic simulation data, which has a statistical and/or structural meaning for a researcher or user. A state detection module (SDM) 102 identifies and extracts a specific state using the abnormal data separated in ADM. The specific state is a targeted state. A data separation module 103 separates the targeted state data from the n th layer data using the targeted state detected in SDM. The system iteratively performs a method processing data in each successive layer of data (i.e., processing a $(n+1)$ th layer) using untargeted data in the n th layer, outputting a targeted state and its data 105 for each iteration. The system may stop iterating when the untargeted state data meets a stopping criteria.

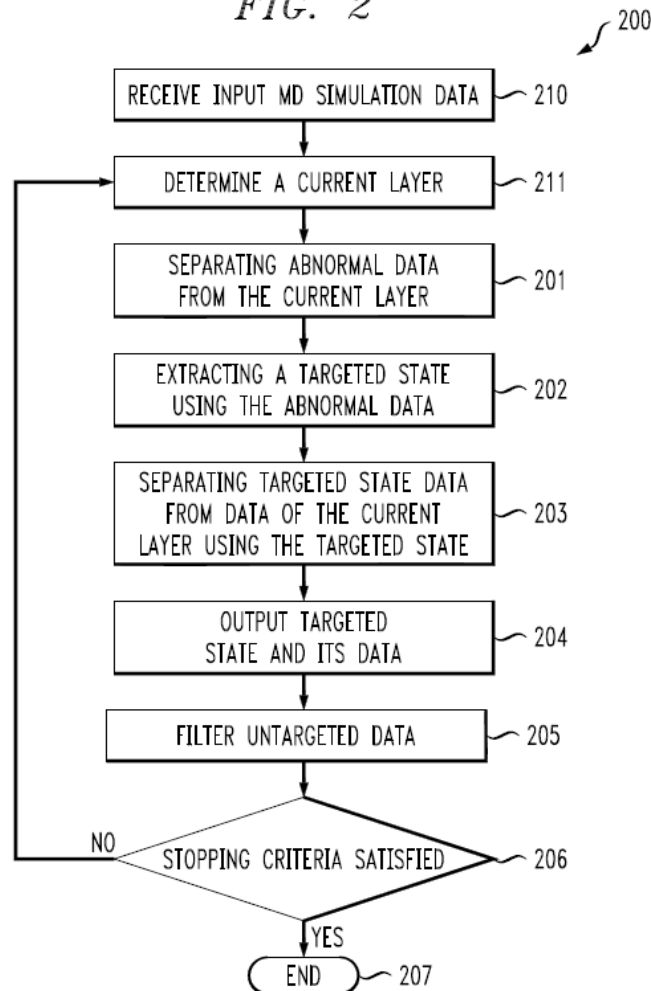
FIG. 1



- 7 Figure 2 illustrates a method 200 for finding unknown molecular dynamics states comprising separating abnormal data from a current layer of data 201, extracting a targeted state from the abnormal data 202, and separating targeted state data from the n th layer data using the extracted targeted state 203. Method 200 iterates through n layers of data, processing the $(n+1)$ th layer using untargeted data in the n th layer. That is, a current layer is processed using the untargeted data from the

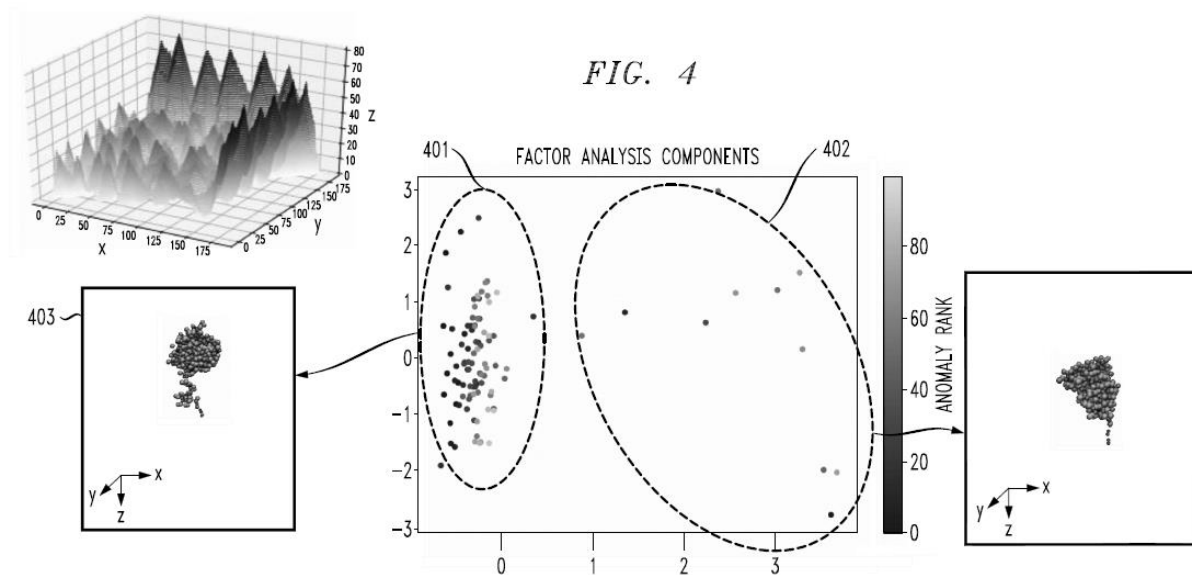
previous layer. At each iteration the method outputs 30 the targeted state and its data at 204, determines whether there are additional layers 205-206, and if so increments the current layer 211 (e.g., current layer $n = n+1$) before starting a next iteration, and if not, ends the simulation 207.

FIG. 2



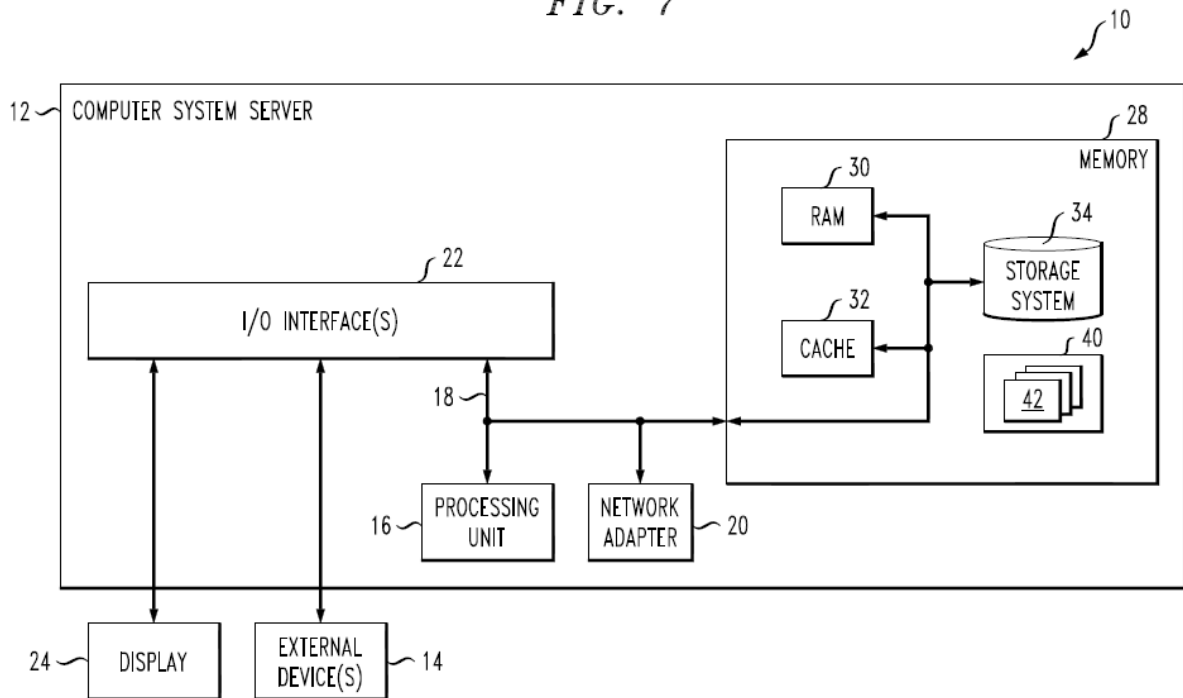
- 8 The extraction of the targeted state from the abnormal data 202 includes sampling the abnormal data to determine targeted samples, and inferring (e.g., by statistical inference) the targeted state from the targeted samples. Thus, the targeted state is determined from the abnormal data.
- 9 Referring to Figure 4 and the state detection module (SDM) 102, the SDM identifies and extracts a specific state (the targeted state) using the abnormal data separated by the ADM. The SDM extracts the targeted samples from abnormal data, the targeted samples exemplifying the targeted state. The SDM utilizes a clustering algorithm to find the targeted state 401 based on the identification of the targeted samples among the abnormal data. The SDM can use a factor analysis to find the targeted state (e.g., Ras proteins with an elongated farnesyl group, which are used in cancer research, see image 403). The untargeted data 402 is identified as data not statistically relevant to the targeted data in the current iteration (ith iteration). The untargeted data of the abnormal samples from block 205 is reused as input for next

iteration ($i+1$ th iteration) (see block 211). Accordingly, layers are determined iteratively according to the method of FIG. 2.



- 10 As shown in Figure 7 below, a system 12 performs an iterative method of finding unknown molecular dynamics states and corresponding samples. The system comprises a communication interface 22, a processor 16 and a memory 28. The communication interface 22 receives molecular dynamics data. The molecular dynamics data simulating movement of particles. The processor 16 determines a current layer of data from the molecular dynamics data, separates abnormal data from the current layer of data, extracts a targeted state using the abnormal data, and separates targeted state data from the current layer of data using the targeted state extracted using the abnormal data. The memory 28 stores the targeted state and its data derived from the molecular dynamics data.

FIG. 7



11 The latest set of claims filed with attorney's letter dated 7 March 2024 has seventeen claims including three independent claims directed to a method of finding an unknown molecular dynamics state (claim 1), a non-transitory computer readable medium (claim 9) and a system configured to perform an iterative method of finding unknown molecular dynamics states and corresponding samples (claim 16) which are set out below:

1. A method of finding an unknown molecular dynamics state comprising:
 - receiving input molecular dynamics simulation data;
 - determining a current layer of data from the input molecular dynamics simulation data;
 - separating abnormal data from the current layer of data;
 - extracting a targeted state using the abnormal data, wherein the extraction of the target state includes sampling the abnormal data to determine targeted samples, and inferring the targeted state from the targeted samples;
 - separating targeted state data from the current layer of data using the targeted state,
 - wherein the method iterates through a plurality of layers of the input molecular dynamics simulation data, wherein at each iteration the method processes a next layer comprising untargeted data from a prior layer; and
 - outputting the targeted state and the targeted state data from each iteration.

9. A non-transitory computer readable medium comprising computer executable instructions which when executed by a computer system cause the computer to perform the method for finding an unknown molecular dynamics state comprising:
 - receiving input molecular dynamics simulation data;

determining a current layer of data from the input molecular dynamics simulation data;
separating abnormal data from the current layer of data;
extracting a targeted state using the abnormal data, wherein the extraction of the target state includes sampling the abnormal data to determine targeted samples, and inferring the targeted state from the targeted samples;
separating targeted state data from the current layer of data using the targeted state,
wherein the method iterates through a plurality of layers of the input molecular dynamics simulation data, wherein at each iteration the method processes a next layer comprising untargeted data from a prior layer; and
outputting the targeted state and the targeted state data from each iteration.

16. A system configured to perform an iterative method of finding unknown molecular dynamics states and corresponding samples, the system comprising:
a communication interface configured to receive molecular dynamics data, the molecular dynamics data simulating movement of particles;
a processor configured to determine a current layer of data from the molecular dynamics data, separate abnormal data from the current layer of data, extract a targeted state using the abnormal data, separate targeted state data from the current layer of data using the targeted state extracted using the abnormal data, wherein the extraction of the target state includes sampling the abnormal data to determine targeted samples, and inferring the targeted state from the targeted samples, and output the targeted state and the targeted state data from each iteration; and
a memory configured to store the targeted state and its data derived from the molecular dynamics data,
wherein the processor is further configured to iterate through a plurality of layers of the input molecular dynamics simulation data, wherein at each iteration the processor processes a next layer comprising untargeted data from a prior layer.

The law

- 12 The examiner has raised an objection under section 1(2) of the Patents Act 1977 that the invention is not patentable because it relates inter-alia to one category of excluded matter. The relevant provisions of this section of the Act are shown in bold below:

1(2) It is hereby declared that the following (among other things) are not inventions for the purposes of this Act, that is to say, anything which consists of –

(a) a discovery, scientific theory or mathematical method;

(b) a literary, dramatic, musical or artistic work or any other aesthetic creation whatsoever;

(c) a scheme, rule or method for performing a mental act, playing a game or doing business, or **a program for a computer**;

(d) the presentation of information;

but the foregoing provision shall prevent anything from being treated as an invention for the purposes of this Act only to the extent that a patent or application for a patent relates to that thing as such.

- 13 The examiner and the applicant agree that the assessment of patentability under section 1(2) is governed by the judgment of the Court of Appeal in *Aerotel*¹, as further interpreted by the Court of Appeal in *Symbian*².
- 14 In *Aerotel*, the court reviewed the case law on the interpretation of section 1(2) and approved a four-step test for the assessment of what is often called "excluded matter". In *Emotional Perception (CoA)*³, the Court of Appeal confirmed (at [31]) that the four steps of the *Aerotel* test are:

Step one: properly construe the claim

Step two: identify the actual contribution (although at the application stage this might have to be the alleged contribution)

Step three: ask whether it falls solely within the excluded matter

Step four: If the third step has not covered it, check whether the actual or alleged contribution is actually technical.

- 15 Subsequently, the Court of Appeal in *Symbian* made clear that the *Aerotel* test is not intended to provide a departure from the previous requirement set out in case law, namely that the invention must provide a "technical contribution" if it is not to fall within excluded matter. The *Aerotel* test has subsequently been endorsed by the Court of Appeal in its decisions in both *HTC*⁴ and *Lantana*⁵.
- 16 Lewison J (as he then was) in *AT&T/CVON*⁶ set out five signposts that he considered to be helpful when considering whether a computer program makes a technical contribution. In *HTC* the signposts were reformulated slightly in light of the decision in *Gemstar*⁷. The signposts are:

i) Whether the claimed technical effect has a technical effect on a process which is carried on outside the computer.

¹ *Aerotel Ltd v Telco Holdings Ltd and Macrossan's Application* [2006] EWCA Civ 1371, [2007] RPC 7

² *Symbian Ltd's Application* [2008] EWCA Civ 1066, [2009] RPC 1

³ *Comptroller-General of Patents, Designs and Trade Marks v Emotional Perception AI Ltd* [2024] EWCA Civ 825

⁴ *HTC Europe Co Ltd v Apple Inc* [2013] RPC 30

⁵ *Lantana v Comptroller-General of Patents, Designs and Trade Marks* [2014] EWCA Civ 1463

⁶ *AT&T Knowledge Venture/CVON Innovations v Comptroller General of Patents* [2009] EWHC 343 (Pat)

⁷ *Gemstar-TV Guide International Inc v Virgin Media Ltd* [2010] RPC 10

ii) Whether the claimed technical effect operates at the level of the architecture of the computer; that is to say whether the effect is produced irrespective of the data being processed or the applications being run.

iii) Whether the claimed technical effect results in the computer being made to operate in a new way.

iv) Whether the program makes the computer a better computer in the sense of running more efficiently and effectively as a computer.

v) Whether the perceived problem is overcome by the claimed invention as opposed to merely being circumvented.

- 17 Paragraph 41 of *AT&T/CVON* emphasises that consideration of the signposts should properly reflect both stages 3 and 4 of the *Aerotel* approach:

If there is a technical effect in this sense, it is still necessary to consider whether the claimed technical effect lies solely in excluded matter.

- 18 The signposts are merely guidelines; although they provide a useful aid in assessing the technical character of a claimed invention, they were not intended to provide a definitive test (as Lewison LJ's obiter remarks in paragraph 149 of *HTC* make clear). Several judgments have emphasised this point - John Baldwin QC (sitting as a Deputy Judge) in *Really Virtual*⁸ noted that the signposts, although useful, are no more than signposts and that there will be some cases in which they are more helpful than in others. Kitchin LJ made similar remarks in paragraph 51 of *HTC* that their usefulness does not mean they will be determinative in every case.

Arguments and analysis

- 19 The examiner maintains that the claims define an invention which consists of a program for a computer. His position is set out in his examination and pre-hearing reports. Detailed arguments against the examiner's position are contained in the applicant's responses to the examination reports through their attorney. Taking all these arguments into account, I must determine whether the claimed invention relates solely to excluded subject matter under section 1(2)(c) of the Patents Act 1977 as a program for a computer as such.

Step 1: Properly construe the claims

- 20 The first step of the test is to construe the claims. In his pre-hearing report, the examiner has explained that he considers the claims to be clear and can be construed as written. As explained by the examiner in his pre-hearing report:

The claims relate to the processing of molecular dynamics (MD) data. MD is a method of simulating the motion of atoms and molecules which can be used to understand and predict the behaviour of complex systems. Given the complexity of the data processing involved in the claimed method, the method is implicitly computer-implemented. The steps of the method generally relate to

⁸ *Really Virtual Co Ltd v UK Intellectual Property Office* [2012] EWHC 1086 (Ch)

the processing of the MD data and the output of the results by a computer program.

- 21 I do not think understanding the meaning of the claims presents any real problem and I consider them to be clear. There is no dispute between the applicant and the examiner as to how the independent claims should be construed.
- 22 Whilst independent claims 1, 9 and 16 relate to different categories of protection, they do not differ in substance so they will stand or fall together.

Step 2: Identifying the actual or alleged contribution

- 23 Jacob LJ outlined the considerations to be applied when identifying the contribution made by the claims in paragraph 43 of *Aerotel* – the critical factors for the examiner to consider are emphasised:

“it is an exercise in judgment probably involving the problem said to be solved, how the invention works, what its advantages are. What has the inventor really added to human knowledge perhaps best sums up the exercise. The formulation involves looking at substance not form – which is surely what the legislator intended.”

- 24 The examiner has offered an amended version of the contribution in his pre-hearing report. The examiner has identified the actual contribution made by the present invention to be:

The contribution is a computer-implemented method of finding unknown molecular dynamics states in a set of MD simulation data, wherein the method comprises iterating through layers of data, each iteration determining abnormal data of a layer, and eliminating data that is unrelated to the abnormal data of the layer. Statistical analysis is then used to infer new information relating to rare, but statistically relevant states of the molecule. Finding rare states may result in a greater understanding of the physical functionality of the molecule. Paragraph 18 of the description gives one example of using these rare states to identify new drug targets.

- 25 The applicant has not disagreed with the examiner’s view of the contribution and has not provided an alternative definition of what they believe to be the contribution made by the proposed invention. I am content to accept the contribution identified by the examiner.

Steps 3 and 4: Does the contribution fall solely within excluded matter/is it technical?

- 26 What I must now decide is whether the contribution identified above relates solely to a program for a computer as such. This corresponds to step three of the *Aerotel* test.
- 27 In this case, the arguments concerning whether the invention is excluded are very much wrapped up with the question of whether the contribution is technical. Given that, I have considered the third and fourth steps together.
- 28 In this case, it is clear that the arrangement of hardware used to implement the invention is immaterial to the working of the invention. The hardware is all

conventional hardware. Given this point, the contribution must therefore be viewed as being embodied purely in a computer program. Whilst the invention undoubtedly uses a computer program for its implementation, the mere fact that the invention is affected in software does not mean that it should be necessarily excluded as a program for a computer as such. What matters is whether or not the program provides a technical contribution.

- 29 As explained in the examiner's pre-hearing report, the arguments of the examiner and the applicant are centred on the first signpost and the interpretation of the precedent in *Vicom*⁹, *Halliburton*¹⁰ and *Emotional Perception (HC)*¹¹.
- 30 At this point it is useful to consider the *AT&T/CVON* signposts as they are a helpful aid when considering whether a computer program makes a technical contribution. The examiner has made reference to the signposts in his examination reports. In his assessment of the five signposts the examiner determined that the contribution failed to satisfy any of the signposts. I note that the applicant has not explicitly referred to the signposts, but has discussed in detail some of the specific cases on which these signposts are based, which I will consider in turn.

Signpost (i)

- 31 The first signpost asks whether the claimed technical effect has a technical effect on a process which is carried on outside the computer. As part of my consideration of the first signpost, I will also consider the legal precedent of *Vicom*, *Halliburton*, and *Emotional Perception (HC)* in identifying whether the claimed computer-implemented invention results in a technical effect outside the computer.
- 32 The applicant's argument is that the contribution of the present claims is technical in nature because the data processing which derives the new information is analogous to the filtering of the image in *Vicom*. The examiner maintains that the result of *Vicom* does not apply to the data in this case because the information derived by the present method is not related to a technical process. In *Vicom*, the image filtering was itself said to be technical in nature and thus the examiner argues that the present case differs because the derived information is comparatively abstract. The knowledge about the molecule has no defined technical purpose.
- 33 In *Vicom*, it was concluded that the claim was not excluded because the mathematical method which underlay the invention was being used in a technical process which was carried out on a physical entity by technical means. The invention in *Vicom* concerned a method of image convolution which involved repeated selection and application of convolution filters using a mathematical error-minimisation technique. As the court explained in *AT&T/Cvon* (see [18]), the Board held that the inventive algorithm in *Vicom* was more than a program for a computer "as such" because:

⁹ *Vicom Systems Inc T0208/84 [1987]*

¹⁰ *Halliburton Energy Service's Inc's Application [2012] RPC 12*

¹¹ *Emotional Perception [2023] EWHC 2948 (Ch)*

“... what was claimed was not the computer program at all, but the process of manipulating the images. That process was a technical process and hence made a technical contribution.”

- 34 In my view, the result of the claimed invention is processing of data to identify MD states which, whilst the method was previously unknown, does not make any change to the physical system. Whilst this can lead to the identification of new drug targets, this is just one example of the use for the identified state structures, MD simulations being widely applicable across various fields. It is also acknowledged that it is more than just searching the data for data objects, but constructs these objects using selected points from the starting data. However I consider that, whilst the present application provides a new way of identifying rare events and anomalies in MD simulation data, it does not go as far as actually providing a real-world application in a technical field. There is nothing analogous to the digital image, which is processed and changed in *Vicom* and therefore I do not consider that there is an analogous technical process in the present application.
- 35 The contribution made by the claimed invention has also been compared to the drill bit design of *Halliburton*. The applicant noted that the drill bit design in *Halliburton* is a set of data and that the related claim does not extend to the actual production of the drill bit. Thus, it was argued by the applicant that the output data of the present method should not be excluded merely for resulting in the output of a dataset. It was also noted that the information output by the method of the present claims can be useful in the technical field of drug design, similar to how the drill bit design of *Halliburton* can be useful in the technical field of drill production. The examiner disagrees that the two are analogous: the drill bit design implicitly is used to produce a drill of the determined specifications, but the MD state information does not necessarily imply a specific use case. Although the MD data may be used to identify drug targets, this information alone does not provide a direct path to a new drug design. It would take significant effort on the part of the skilled person to take the information derived from the inventive method and go on to design a drug using that information. Without a defined and clear industrial purpose, the information derived by the inventive method is academic rather than technical.
- 36 I do not consider the contribution made by the claimed invention to be analogous to the contribution made by *Halliburton*. Similar to *Vicom*, which produces a new image, *Halliburton* produces a new drill bit design. The present invention is not designing anything new, but is processing data to identify already existing MD states. Whilst these may be useful in identifying new drug targets, the contribution is not a design of a new drug – that is a subsequent process. Whilst *Halliburton* didn't have to have the final step of actually manufacturing the drill bit, it did clearly define how to design it. As argued by the examiner, even if the claim were limited to this purpose, it would take significant effort on the part of the skilled person to take the information derived from the inventive method and go on to design a drug using that information. Without a defined and clear technical purpose the contribution does not provide a means of designing anything new. The data describes a real, physical system which, whilst previously unknown, already existed and has not been designed or changed by the invention.
- 37 The applicant has also argued that the output of the present method escapes exclusion because “the outputting of a file selected or generated in a technical way

... constitutes a technical contribution” from the judgement in *Emotional Perception (HC)*.

- 38 The examiner considers the present invention to differ significantly from the circumstances of *Emotional Perception (HC)*. The discussion in *Emotional Perception (HC)* of the file transfer follows a lengthy discussion of the other details of the claimed invention, and the judgement in paragraph 76 specifically notes that “the ANN has certainly gone about its analysis and selection in a technical way”, and that the exclusion is avoided in *Emotional Perception (HC)* due to the “purpose and method”. In the present case, the examiner does not consider that the targeted state information is generated in a technical way, so the output of the targeted state information does not in itself demonstrate a technical contribution.
- 39 It is noted that, since the latest correspondence on file, this judgement has been overturned, but it is important to consider the reasoning for that and how it may apply in this case. There is acknowledgement in the Court of Appeal judgement that selecting a file could be technical if made in a technical way, but it was noted that provision of a recommendation message is the presentation of information – which is also unpatentable subject matter, unless it involves a technical contribution. Further making a better recommendation based on semantic rather than technical criteria is not technical.
- 40 In this case I do not consider that the invention is providing a better recommendation in the same way that the invention of *Emotional Perception* was. The user is being presented with the output of statistical analysis, representative of an unknown MD state, which is very different from making a better recommendation of a music file to a user based on semantic similarities. Whilst the output is not based on semantic or aesthetic considerations, neither is it a file, such as a music file which can be played, but rather a target state and target state data. Whilst this may involve constructing a new data object, it is nevertheless the manipulation of the data to provide information about a real-world system, rather than something tangible selected for, delivered to and used by the user in the way that a digital image or music file is. I do not therefore consider that analogy is helpful in determining whether the present invention provides a technical output in a technical way. Therefore, I do not consider the analogy to the file in *Emotional Perception (HC)* points to a technical effect outside of the computer.
- 41 In considering *Vicom*, *Halliburton* and both the High Court and Court of Appeal judgements on *Emotional Perception*, I have not found the contribution to be analogous with any of these judgements. I do not consider there to be any technical effect having a technical effect on a process which is carried on outside the computer. Therefore, in my view the first signpost is not met and points away from there being a technical contribution.

Signposts (ii)-(iv)

- 42 I agree with the examiner’s assessment of signposts (ii)-(iv) and consider them to not assist the applicant. The contribution of the proposed invention does not address a problem at the architecture/hardware level of a computer, it uses known hardware with any adaptations being made at the application level. The computer does not operate in a new way other than the running of a new program.

43 The applicant has not provided any argument relying on any of signposts (ii)-(iv).

Signpost (V)

44 The fifth and final signposts asks whether the perceived problem is overcome by the claimed invention as opposed to merely being circumvented. The fifth signpost looks at the technical character of an alleged invention by means of the problem addressed. When the problem is a technical one, the alleged invention can be considered to have a technical nature leading to it falling outside the exclusion.

45 Whilst the invention enables previously unknown MD states to be identified and displayed, this is a problem lying in the field of statistical analysis rather than a technical improvement to the computer itself or a real world application lying outside of the computer, as discussed above. Therefore, signpost (v) is not satisfied.

46 The examiner has also discussed Office decisions BL O/130/22 and BL O/1193/23. As I have found the claimed invention to not provide a technical contribution, I do not consider it necessary to discuss these two decisions further here. However, I do consider my decision here to be in line with said decisions.

47 Therefore, I consider the contribution identified above to relate to a program for a computer as such.

Conclusion

48 For all the reasons set out above, I find that the claimed invention is excluded under section 1(2)(c) as a program for a computer as such. I refuse this application under section 18(3).

Appeal

49 Any appeal must be lodged within 28 days after the date of this decision.

Sally Vinall

Patent Examination Group Head