



**Physical Sciences**

## **Computational Life Sciences (CLS)**

**Call for proposals subsidy round 2008**

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# 1 Introduction

**On behalf of the boards of the Netherlands Bioinformatics Centre (NBIC), the Netherlands Genomics Initiative (NGI) and the Netherlands National Computing Facilities Foundation (NCF), the Board of the NWO council for Physical Sciences invites researchers in (bio)informatics, (bio)mathematics, life sciences and other disciplines to submit research proposals for the *Computational Life Sciences Programme*.**

Appendix 1 (of the Dutch version of this call\*) contains guidelines to help you write your proposal.

**NB.** The substance of this call does not differ from that of the previous CLS round (2007), though the wording has been clarified here and there. Please read the entire call carefully.

## 1.1 Organisational background

In 2002, NWO's General Board made available a one-off sum for the launch of a number of new programmes in connection with the NWO *Themes with Talent* strategy. As part of the *Fundamentals of Life Processes* theme<sup>1</sup>, the Computational Life Sciences (CLS) programme was launched alongside already existing programmes, including *Biomolecular Informatics* (BMI) and *Genomics*. NBIC launched its bioinformatics programme *BioRange* in 2005. This and other initiatives have given rise to some important work in the Netherlands on large-scale molecular processes in and between cells, involving (bio)informatics experts and (bio)mathematicians working in collaboration with life scientists.

The 2007/2008 rounds of the Computational Life Sciences programme provide an opportunity for current initiatives to be followed up. The first round (2007) has now closed. Five projects were awarded grants. The organisations that initiated the programme hope that these rounds will enable collaboration between (bio)informatics experts, (bio)mathematicians and life scientists to become structural. The CLS programme therefore ties in well with the NWO Systems Biology theme, which the NWO, NGI and NBIC regard as an important development. The CLS rounds are the first initiative to get underway in the framework of this theme.

Applicants are urged to ensure that the substance of their proposal ties in with current CMS or BMI research, or with research being conducted under NGI and NBIC programmes. For further information on these projects, see section 5.1. The scientific quality and relevance (to the life sciences and physical sciences) of the proposed research will be the deciding factor in granting awards, taking into account the factors discussed in section 4.

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\* In the event of differences of interpretation, the Dutch version of the call will take precedence over the English version.

<sup>1</sup> Under the NWO Strategic Plan 2007-2010, the Fundamentals of Life Processes theme will continue as Systems Biology.

## 1.2 Scientific background

The amount of biological data available continues to increase exponentially. More and more complete genome sequences are being mapped (over 450 are now available) and there is likely to be explosive growth in the amount of data available, given the 2000 or so genome projects that are currently in progress. This treasure trove of information allows experiments to be designed, data collected and patterns identified across entire genomes and between genomes. Examples include the mapping of transcriptome changes in biological ecosystems using microarrays, the identification of genes involved in biological processes using genome-wide RNAi in combination with high-throughput assays for phenotyping, and the cataloguing of protein-protein interactions by means of systematic two-hybrid and pull-down assays. Furthermore, modern proteomic and metabolomic techniques allow the composition of entire biomolecular systems and any changes to be identified. In recent years, a number of publicly accessible databases have also been developed in the life sciences, to store the steadily expanding mass of transcriptome, proteome and metabolome data.

The *model-driven* approach has taken off on a big scale over the past few decades, both supported by and dependent on this growth in biological data. This approach, which is generally based on a quantitative description of the underlying mechanism, has given rise to a broad range of insights into how all kinds of subsystems function, including specific proteins; membrane systems; metabolic, genetic and signal transduction networks; the cytoskeleton; and many other systems and processes occurring at cellular level. On a larger scale, models of tissues and organs can increase our understanding of the dynamics of gene expression patterns; tissue growth and physiology, including the blood supply; the growth of tumours; and the growth of neurons and axons.

Given the availability of large quantities of data, new methods for measuring model parameters and the potential use of models for the efficient collection of new data (model-driven data collection), now is an ideal time to combine the two approaches. Uniting these two often disparate styles of research is therefore one of the goals of the 2007/2008 rounds of the CLS programme.

## 1.3 Research framework

The research theme for the CLS 2008 round (and previously for the 2007 round) is ***biological networks***. This theme, and the research issues associated with it, is explained in this section. A number of examples are also presented to illustrate the kind of studies that are envisaged.

### **Biological networks**

The huge stock of public biological databases and our increased knowledge of cellular networks have led to the development of a broad range of bioinformatics methods that allow researchers to search and analyse databases from a biological perspective (data mining). One key area where further developments are needed is in the integration of these databases with (bio)informatical and (bio)mathematical analysis. The integration of data and methods should give us a new understanding of the structure and workings of biological networks in various conditions or in different cell types and organs. This knowledge, in turn, would allow the dynamics of biological networks to be studied on various temporal and spatial scales (from picoseconds to evolutionary, and from molecular to organism). Innovative (bio)informatical and (bio)mathematical methods are needed for these biological networks to be modelled.

## 1.4 Budget

The financial backers have made a total of EUR 4.82 million available for this programme. This will be used to fund two competitive rounds. Approximately EUR 2.27 million was committed in the 2007 round. Five grants are available in the 2008 round, each worth EUR 460,000.

A small proportion of the budget is reserved for programme activities such as the organisation of symposia, workshops and other knowledge transfer activities. These will tie in with ongoing NWO research being funded under the *Computational Life Sciences* and *From Molecule to Cell* programmes, and with activities running under the NBIC *BioRange* programme.

The Netherlands National Computing Facilities Foundation (NCF) is also participating in this programme, helping to assess proposals that mention a need for calculation or data storage, separately prioritising applications for calculation time according to its procedures, holding workshops for researchers on the use of its facilities and, if desired, evaluating software developed under the programme.

## 2 Aim

### 2.1 Focus of the programme

The studies in this round should contribute to the integration of *data based (bio)informatics research* and *dynamic models*. This implies the development of models that can be used to analyse data from a biological network in such a way that the model describes the properties of the network on various temporal and spatial scales (from picoseconds to evolutionary, and from molecule to organism).

Studies should produce:

1. *New insights into biological networks* by developing new concepts and techniques based on physical science, specifically, in this context, (bio)mathematics and (bio)informatics.
2. *Greater understanding of biology*. Studies should focus on challenging issues in biology.
3. *Scale bridging*. Studies should be based on a multi-scale approach (micro-, meso- and macroscopic level, time, space, dynamics and environment).

Embedding at the interfaces between (bio)informatics, (bio)mathematics and life sciences will be a requirement, and all three scientific disciplines must be represented in the research team.

### 2.2 Types of study: examples

The aim of this round is to provide scope for proposals designed to increase our understanding of biological networks. A number of examples of the type of research defined in the previous sections are given below to serve as inspiration.

#### 2.2.1 Simulation of biological regulatory networks

One of the most spectacular developments in biology was the discovery in the 1980s of genes and gene networks, which regulate growth and shape in organisms. The modelling of this type of process requires different modelling techniques to be linked at various spatial and temporal scales (meso-scale modelling). Various spatio-temporal gene expression data must be linked in order to develop these models. The availability of techniques for deriving model parameters from these data is of great importance. Development of simulation models can give rise to a focused and efficient manner of data collection (model-driven data collection).

One good example of this is the quantitative heart model, where integration has been achieved between the molecular level (ion channels, hormone receptor, signal transduction systems), the cellular level (various types of cell in the heart and their connections), and the tissue level.

#### 2.2.2 Integration of biological networks

Our knowledge of metabolic and gene regulation networks has expanded enormously since the advent of functional genomics. Genome-scale metabolic models have been developed, showing the relationships between genes, their protein products and the reactions that these proteins can catalyse. Regulation networks have been reconstructed on the basis of bioinformatics, co-expression of genes and other high-throughput techniques such as transcription factor binding studies. However, the integration of these networks and the associated data still presents problems, and

requires collaboration between biologists (physiology, regulation), computer scientists (data analysis and integration) and mathematicians (graph theory, control theory).

For example, time-scale analysis and computer simulations can show us which enzyme activities in a network are regulated metabolically, and which enzymatically. Stoichiometry and graph analysis can reveal the role of network topology and flux distributions in the organisation of operons and regulons, for example.

### 2.2.3 Dynamic properties of network motifs

Biological networks, such as the regulation of genes, signal routes or neural synapses, are representations of large-scale dynamic systems. We can obtain more knowledge of the organisational principles behind biological networks by becoming aware of the interaction between network structures and system dynamics.

The structural properties of biological networks have already been extensively studied. However, little attention has so far been paid to their dynamic properties. One of the few examples of such a study was presented by Prill et al<sup>2</sup>. Using an extensive computational analysis, they showed that dynamic properties – such as stability and robustness in the face of small perturbations – are strongly correlated with the relative enrichment of small partial networks (or network motifs) in various biological networks. The results of this work suggest that robust dynamic stability might be a driving mechanism behind the non-random structure of biological networks.

### 2.2.4 Evolution of network structures

Besides describing the dynamics, as in the previous example, it would also be interesting to explore the evolution of such network structures using evolutionary simulations. One might consider the extent to which the observed network structures may be a side effect of the mutation dynamics (duplication, deletion of genes or chromosome segments), or one might use evolutionary models to establish under what conditions the dynamic properties of such network patterns are indeed selected, and the extent to which mutation dynamics plays a role in this.

### 2.2.5 Biochemical and mechanical interactions in biological networks

The interaction between mechanical load and biological function is crucial to many biomedical questions. There is often a huge discrepancy in scale. In a bone, for example, the length scale of the load and that of the tubular microstructure differ by many orders of magnitude, and vibrations at the scale of seconds and milliseconds can lead to structural changes in the following weeks and months.

Synthetic heart valves, by way of another example, develop enough strength only if they are exposed to a mechanical load during growth. A good understanding of these processes requires an integrated approach, in which the biochemistry is depicted spatially and can be manipulated, while the mechanics are introduced biochemically. The potentially huge differences in spatial and temporal scales make this a scientifically and computationally challenging field of research.

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<sup>2</sup> Prill RJ, Iglesias PA, Levchenko A (2005) Dynamic Properties of Network Motifs Contribute to Biological Network Organization. *PLoS Biol* 3(11): e343 [doi:10.1371/journal.pbio.0030343](https://doi.org/10.1371/journal.pbio.0030343)

### 2.2.6 Derivation of biological networks using machine learning techniques

Signal routes are generally pieced together from studies of the individual components of the route derived from various experimental systems. Although the routes are often conceptualised as separate entities that respond to different triggers, it is becoming clear that the interactions between the routes and other properties of these networks cannot be explained by studying individual routes in isolation. A global multivariate approach is needed to understand normal cellular response and how it can be disrupted by disease.

One example of a multivariate approach is the use of Bayesian networks – from the world of machine learning– to model complex systems such as signal routes, mainly because such networks can represent probabilistic dependencies between the various interacting components. This machine learning approach allows the causal influences in cellular signal networks to be identified.

### 2.2.7 Biological networks in multi-unit interactions in cells and tissues

Biological networks are essential to an understanding of how a living cell or collection of cells functions. The problem is that many different elements interact in many different ways. Within a cell, function is determined by a large number of proteins and other functional molecules, and the resulting processes are not easy to understand on the basis of the structure and properties of each of the molecules involved.

Likewise, cell differentiation gives rise to networks of different cells with different properties that all interact with each other in different ways, producing complexes (such as organs) that have new qualitative properties. Important new insights could be obtained by studying the immune system, the nervous systems, developmental biology, membrane processes and the cytoskeleton of cells.

### 2.2.8 Genome evolution

The steadily growing quantities of data on entire genomes, expression and protein interaction mean that it should be possible to identify evolutionary patterns in the data. Important questions include the evolutionary development and preservation of 'modules', the changes in regulation networks, chromosome structure, the co-evolution of 'orthologous groups' etc.

It would be an interesting challenge to study the evolutionary processes underlying these issues using evolutionary simulation models (computational evolution). Such an approach might for example be used to demonstrate that transposon dynamics combined with evolution in a variable environment can lead to chromosome structures which facilitate short-term adaptation, as suggested by data from evolution experiments in yeast. Another example might study the extent to which co-evolution of antibiotic-producing bacteria can lead to the sudden increases in transcription regulation observed in the data.

## 3 Guidelines for applicants

### 3.1 Who can apply?

Research proposals may be submitted by researchers at Dutch universities, and at NWO and KNAW institutes. The proposal should be submitted by one researcher (the main applicant) on behalf of a team consisting of researchers from one or more research institutions. Simultaneous submission of identical or highly similar proposals is not permitted. Nor may research proposals that are already being implemented or are in the process of being assessed be submitted to one of the funding organisations.

You should submit a copy of your proposal to the director or dean of your institution. Once you have submitted a proposal, the programme office will assume that you have informed your institution, and that the university or institute accepts the grant terms and conditions applying to this competition. You should also:

- have at least a *doctoraal* or *ingenieur* or similar qualification;
- have sufficient research experience;
- be in a position to be effectively involved in the research for which a grant application is being submitted throughout the period for which the grant is being requested.

The organisations behind the programme would particularly welcome proposals from female researchers.

### 3.2 What can be applied for?

#### 3.2.1 Research grants

Research proposals must be based on a grant of € 460,000, at least € 360,000 of which must be intended for two or three research positions. A margin of 10% above or below this amount would also be acceptable, on condition that it is made clear that the applicant institution will be liable for any budget overrun.

The grant may be used for:

- Full-time research students (OIOs) and two- or three-year post-docs. An individual bench fee will be awarded to each research assistant or post-doc to (fully or partially) cover costs such as travel expenses and the printing of their thesis.
- University lecturers/senior university lecturers. If lecturers devote more than 75% of their working time to the research activities, their entire salary may be paid from the grant. If more than 25% of their time is spent on other activities, only the salary for the proportion of their working time spent on the research may be paid from the grant. A university lecturer/senior university lecturer must be allocated to the research for at least 0.4 FTE. Grants will not be awarded for fewer hours.
- Extension of the research duties of incumbent university/senior university lecturers with hours amounting to at least 0.4 FTE. In certain exceptional cases, a grant may be awarded for this purpose, as it is easier to attract new teaching staff than new researchers. If you are interested in this option, please contact the programme office.

Grants may also be requested, solely in combination with a research position, and lasting no longer than this position, to cover the costs of:

- Technical staff and programmers to provide technical support (e.g. experimental work) specifically related to the programme. Technical support as such may not be requested.
- Project-related equipment/software/experiments, provided their total costs fall between € 5000 and € 110,000. The equipment must be intended exclusively for the project described in the proposal. The need for the equipment and its relationship to the project must be thoroughly substantiated. Equipment/experiments costing more than € 40,000 must also be properly embedded in the research. Equipment/software costing less than € 5000 will be regarded as part of the institution's infrastructure and will not therefore be eligible. In the event that the research involves animal testing, a statement of compliance with the guidelines on animal testing must be submitted.
- Travel expenses for the research positions in the application, in so far as they are not covered by the bench fee. The need for the project, particularly for the research positions, must be well substantiated.
- Travel and accommodation costs for guest researchers from other countries whose input is relevant to the research. Here, too, arguments must be presented in support of their involvement.

### 3.2.2 Access to national computer facilities

The Netherlands has one of the fastest computer networks in the world, and sophisticated central computing facilities, including the National Supercomputer with a large memory and rapid processor connections, and LISA (the *Nationaal Rekencluster*), which can perform large numbers of independent calculations (e.g. parameter studies). In the course of 2008 the National Supercomputer will reach a capacity of over 60 Tflop/s, putting it among the leading systems in Europe. The system is financed and monitored by the Netherlands National Computing Facilities Foundation (NCF). A number of other advanced facilities are also available, including the CAVE visualisation environment, and a data storage centre. All facilities are administered by SARA in Amsterdam and Almere. Time may be requested on these computing facilities and on the CAVE as part of a research proposal. A special application form is available for the purpose.

## 3.3 When can applications be submitted

The deadline for the submission of proposals is **on 15 October 2008, 12.00H.**

## 3.4 Drawing up an application

All proposals should be written in English so that foreign reviewers can be consulted. The proposal should be a discrete document, and reference to any internal documents should therefore be avoided. Only references to the "open literature" are permitted. Should reference to a preprint prove unavoidable, applicants are requested to enclose a copy (in electronic form) so that the assessors can refer to it. Further information on how proposals should be structured is enclosed.

## 3.5 Submitting an application

Applicants should use **Iris**, NWO's electronic grant application system. Please see <https://www.iris.nwo.nl> for instructions on how to use the system. An application should consist of two parts: a **factsheet** listing key data on both the applicant and

the proposal,<sup>3</sup> and the **research proposal** itself. The factsheet should be completed and submitted electronically using Iris. The research proposal should be sent at the same time as a PDF attachment.

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<sup>3</sup> The **factsheet** must be completed using only ASCII symbols (plain text). It will not therefore be possible to use formulae, italics etc. They may, however, be used in the **research proposal**.

# 4 Assessment procedure

## 4.1 Procedure

### 4.1.1 Official admissibility of applications

The programme office will declare an application admissible if it meets the following requirements:

- It must be submitted by a researcher at a recognised scientific research institution.
- It must comply with the objectives of the programme.
- It must be in the required form, complete, and the applicant must have responded to any request for further information.
- The amount applied for must fall within the specified range.
- It must be submitted through Iris – NWO's electronic grant application system.
- It must be submitted by the deadline.

If an application does not meet all the criteria, the programme office will contact the main applicant. Major shortcomings will lead to rejection of the application.

### 4.1.2 Suitability Check

Research proposals that meet the above criteria will be further processed and assessed by an international assessment committee. Prior to the scientific assessment of the proposal, the assessment committee will establish whether the proposed research meets the following criteria:

- It must fall within the research framework of this round as set out in section 3.
- It must address the three points in section 3.2.
- The scientific disciplines (bio)mathematics, (bio)informatics and life sciences must be represented in the research team.

The assessment committee reserves the right to advise the Physical Sciences Board to reject applications (at this stage) if they do not meet the above criteria. Any applicants experiencing doubts prior to submission as to whether their proposal meets the criteria are advised to contact the programme secretariat. Research proposals that meet the above criteria will be further processed and assessed.

### 4.1.3 Scientific Assessment

In assessing applications, the assessment committee will draw on the advice of independent experts in the Netherlands or abroad ("reviewers"). Applicants will be given the opportunity to suggest up to three potential reviewers.<sup>4</sup> Please supply the full name, title(s), affiliations, gender and email address of potential reviewers. Members of the assessment committee (or others) may also suggest reviewers. The programme office is responsible for approaching reviewers.

Applicants will be given the opportunity to submit a brief response (in no more than 500 words) to the reviewers' comments (counterarguments). Counterarguments

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<sup>4</sup> Applicants may also (but are not obliged to) indicate up to three individuals who may not act as reviewers. To guarantee confidentiality, you are requested not to include these names in your application, but to inform the programme office separately by email.

must be received by email at the programme office within a week of the reviewers' comments being dispatched. Late or excessively long responses will be declared inadmissible and will not be considered in the assessment. If the assessment committee judges the tone of the response to be unbusinesslike, it will be disregarded.

The assessment committee will set an order of priority on the basis of the proposal, the reviewers' comments, the applicants' counterarguments and their own scientifically-based views, in so far as they do not differ from the referees' assessment to such an extent that the applicant must be asked to supply counterarguments. The assessment committee will also issue written recommendations on the proposal.

The Netherlands National Computing Facilities Foundation (NCF) will help assess proposals that mention a need for computing or data storage facilities.

#### 4.1.4 Decision-making

The Physical Sciences Board will decide on the allocation of grants, on the basis of the assessment committee's recommendations. Representatives of NBIC and NGI will be invited to assist in the decision-making. The Board is authorised to reduce the budget available in this round, on the advice of the assessment committee or otherwise, depending on the quality of the proposals received. The Board is also responsible for ensuring the proper implementation of the research programme.

**NB** The funding organisations in this round have made the grant budget available to boost collaboration between (bio)informatics, (bio)mathematics and life sciences. They therefore regard it as important that the research be carried out as quickly as is realistically possible. Under the conditions attaching to the budget, research in this round must commence **within six months** of any grant being awarded. Any projects that do not commence by this deadline will forfeit their grant. All those working on projects must begin their activities in accordance with the project plan. Applicants are therefore advised not to submit proposals in areas where it is unclear whether it will be possible to find staff to perform the research. Applicants are in fact advised to take on senior researchers such as post-docs or (incumbent) university lecturers/senior university lecturers.

## 4.2 Criteria

Applications will be assessed on the basis of their **relevance to the physical sciences (in this case computer science and mathematics) and to the life sciences**. Both sets of criteria carry equal weight.

The scientific quality of the proposals will also be assessed, on the basis of the following seven properties:

- The originality of the research question and method.
- The importance and urgency of the proposed research.
- The clarity of the proposal.
- The programme of work and its feasibility.
- The competence and demonstrable multidisciplinary nature of the research team that is to carry out the proposed research.
- The allocation of the grant requested in relation to the aim of the research.
- The innovative nature of the proposal, either in the sense of a new application of existing techniques and methods, or in the development of new techniques.

In assessing applications, the assessment committee will draw on the advice of independent experts in the Netherlands or abroad ("reviewers"). Applicants will be given the opportunity to suggest up to three potential reviewers.<sup>5</sup> Please supply the full name, title(s), affiliations, gender and email address of potential reviewers. Members of the assessment committee (or others) may also suggest reviewers. The programme office is responsible for approaching reviewers.

Applicants will be given the opportunity to submit a brief response (in no more than 500 words) to the reviewers' comments (counterarguments). Counterarguments must be received by email at the programme office within a week of the reviewers' comments being dispatched. Late or excessively long responses will be declared inadmissible and will not be considered in the assessment. If the assessment committee judges the tone of the response to be unbusinesslike, it will be disregarded.

The assessment committee will set an order of priority on the basis of the proposal, the reviewers' comments, the applicants' counterarguments and their own scientifically-based views, in so far as they do not differ from the referees' assessment to such an extent that the applicant must be asked to supply counterarguments. The assessment committee will also issue written recommendations on the proposal.

The Netherlands National Computing Facilities Foundation (NCF) will help assess proposals that mention a need for computing or data storage facilities.

### 4.3 Committees

The CLS programme committee, made up of experts from various research institutions, is responsible for guiding the scientific content and for the academic coordination of the programme. Its tasks include monitoring the progress of ongoing research projects, producing progress reports and promoting knowledge transfer. A representative of NBIC advises the programme committee, to ensure that the research ties in with NBIC programmes and activities. The programme committee will receive administrative and policy support from a programme office at NWO Physical Sciences.

Applications are assessed by an international assessment committee consisting of independent foreign experts. None of the members may have any involvement with an application, in accordance with the NWO code of conduct on conflicts of interest. The committee assesses and prioritises the research proposals, and produces a written report on the applications.

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<sup>5</sup> Applicants may also (but are not obliged to) indicate up to three individuals who may not act as reviewers. To guarantee confidentiality, you are requested not to include these names in your application, but to inform the programme office separately by email.

## 5 Other information

### 5.1 Contact

For further information, please contact the CLS programme office:

- Yvette Tuin
- tel. + 31 (0)70 344 08 12
- [tuin@nwo.nl](mailto:tuin@nwo.nl)

or

- Dr. Christiane Klöditz
- tel. +31 (0)70 344 05 61
- [kloditz@nwo.nl](mailto:kloditz@nwo.nl)

This call for proposals and information on current CLS and BMI research can be found at [www.nwo.nl/cls](http://www.nwo.nl/cls) and [www.nwo.nl/bmi](http://www.nwo.nl/bmi).

### 5.2 Schedule

Date	Stage of procedure
15 October 2008, 12.00H	Deadline for submission of proposals to project office, via Iris
November 2008	Suitability check
November 2008 to February 2009	Assessment by reviewers
February 2009	Request for rebuttal
March 2009	Assessment committee issues recommendations for order of priority
April 2009	Physical Sciences Board decides which applications should be awarded grants
May 2009	Programme office sends award/rejection letters

Applicants can monitor the progress of the assessment of their project proposal using the project update module in Iris, NWO's electronic grant application system.