

**ab-initio** (computation): computation carried out on the basis of theoretical data, without use of simplifying models adjusted to fit experiments, and intended to be fully predictive

**actinides:** naturally occurring or artificial **radioelements** of atomic number (number of protons in the nucleus) between 89 (actinium) and 103 (lawrencium)

activation: process whereby a stable nuclide transforms into a radioactive nuclide

activation (of a gene): activation of the expression of that gene

**activity:** number of spontaneous nuclear transitions occurring in a given quantity of **radionuclides** over a sufficiently short time span, divided by the length of that time span. Unit of activity is the **becquerel** (Bq), equal to one transition per second

**algorithm:** sequence of logical and mathematical operations required for the carrying out of a computation task

 $\alpha$  helix: structure, in a biological molecule, generated by regular rotation of a polypeptide chain coiling on itself, to form a cylinder where every peptide linkage is hydrogen-bonded to other peptide linkages

**amino acids:** organic molecules forming the building blocks for **proteins**, and containing at least one amino group (NH<sub>2</sub>) and one carboxyl group (COOH)

**amorphization:** complete loss of periodicity, in all three dimensions, in the **crystalline** structure. The long-range orderliness of atom stacking is lost

**antibiotic:** a substance, usually produced by a micro-organism or a plant, that is toxic for some micro-organisms

**assembly** (fuel): assembly of **fuel** elements, loaded into a nuclear reactor as a single unit (comprising, for example, 264 fuel rods, in the case of a **pressurized-water reactor**)

**atomic vibration** (period): the inverse of an atom's vibration frequency around its mean position. It is of the order of 100 femtoseconds (1 fs =  $10^{-15}$  s), and depends on direction, polarization and vibration wavelength

**bases:** in molecular biology, this term refers to the **purines** (adenine and guanine are examples of purine bases) and **pyrimidines** (thymine and cytosine are examples of pyrimidine bases) occurring as constituents of **DNA** and **RNA** 

 $\beta$  sheet: structure in a biological molecule, formed by folding of a polypeptide chain on itself into zigzag ("concertina") pleats, the structure's stiffness being maintained by hydrogen bonds with the peptide linkages in neighboring chains

**biomimetic:** reproducing design concepts or processes inspired from nature

**biosphere:** ensemble of all ecosystems on the planet, comprising all living organisms and the environments they live in

**BWR (boiling-water reactor): one of the two major fami**lies (along with **PWRs**) of common- (light-) water reactors. A BWR uses as coolant and moderator water that is brought to boiling point in the core, under normal operating conditions

**byte:** unit of electronic data storage, equal to 8 bits, allowing storage of 1/8 of a floating-point number, or one character. Most common multiples are: the **kilobyte** (equal to  $2^{10}$  bytes, i.e. 1,024 bytes), **megabyte** (1 MB =  $2^{20}$  bytes or 1,024 kB), **gigabyte** (1 GB =  $2^{30}$  bytes, i.e. 1,024 MB) and **terabyte** (1 TB =  $2^{40}$  bytes, i.e. 1,024 GB)

#### **CAD:** computer-assisted design

**capture** (neutron): absorption of a free **neutron** (by a nucleus) that does not lead to **fission** 

**catalyze:** to accelerate a chemical reaction, without the accelerating substance (an **enzyme**, in biology) itself being modified

**closure laws** or **closure relations:** in a **computation software** program, physical models built up on the basis of analysis of experiments, to express the various transfers of mass, momentum and energy, and forming the source terms for the partial differential equations resolved by the program

**complexation:** formation of a neutral or charged structure (or **complex** compound), containing ions and molecules (organic or inorganic), more infrequently atoms, held by covalent bonds (chemical bond arising from the sharing of one or more pairs of electrons) to a metal ion

complexation site: site where a complex compound will form

**computation software:** drawing up into a software program – often referred to as a *code*, since it is in the form of coded mathematical expressions – of the simplified representation (modeling) of a system or process in order to simulate it

**convection:** motion in a fluid accompanied by heat transport, caused by differences in temperature

**crystal:** structure made up of atoms, ions or molecules forming an array exhibiting three-dimensional regularity

**crystallography** (X-ray): method for the observation of the structure of matter consisting in positioning a sample – a **crystal** as a rule – under a beam of **X-rays** and recording a diffraction pattern on a detector

**deterministic** (numerical method): method where the concept is to substitute for the initial unknown an approximate unknown, only dependent on a finite number of parameters

deuterium: isotope of hydrogen (atomic mass 2)

**dislocation** (in a solid): line defect, displacement of which propagates slippage of one part of the solid against the other. A dislocation line may close upon itself to form a *loop* 

**electronvolt:** unit of energy, defined as the energy acquired by an electron accelerated by a potential difference of 1 volt (1  $eV = 1.6 \cdot 10^{-19}$  joule). Main multiples are: the kiloelectronvolt (keV), megaelectronvolt (MeV) and gigaelectronvolt (GeV)

electrostatic: based on electric charges at rest, subject to no displacement (constant electric field)

**empirical potential:** analytical expression of the potential energy of an assembly of atoms as a function of their positions, dependent on a number of parameters adjusted so as to reproduce measured physical properties

empiricism: method relying on experiment, rather than first principles

**energy bands:** ranges of energies available to electrons in matter

**enrichment:** process whereby, in a given element, concentration of one of its **isotopes** is increased. Outcome of this process is the separation of the end product into two fractions, respectively referred to as enriched and depleted for the isotope of interest. Example: enrichment of uranium in 235-isotope



enzyme: protein catalyzing a specific chemical reaction

equation of state: relation between pressure, volume and temperature in a body

expression (of the genome): production by a gene of an observable phenotype, usually by synthesis of a protein

"fast" reactor: nuclear reactor where presence of materials liable to slow down **neutron** velocity is limited, so that fission is mainly caused by fast neutrons

fatigue: distortion or alteration in state undergone by a material or mechanical component subjected to excessive stresses

**fissile nucleus** or **material**: nucleus (or material) liable to undergo **fission** through **neutron** absorption. Strictly speaking, it is not the so-called fissile nucleus that undergoes fission, but the *compound nucleus* formed subsequent to neutron **capture** 

**fission:** splitting of a heavy nucleus into two parts, accompanied by emission of **neutrons**, radiation, and release of a considerable amount of heat

**flops:** abbreviation for "FLoating-point Operation Per Second"; unit of computational power for a computer for scientific purposes. Most common multiples are: the **gigaflops** (1 Gflops = 1 billion operations per second) and **teraflops** (1 Tflops = 1,000 billion operations per second)

**fuel** (nuclear): material containing **nuclides** whose burning through **fission** in a nuclear reactor allows a chain reaction to be sustained in the reactor

**fusion** (thermonuclear): reaction between two light nuclei leading to production of one nucleus heavier than either of the initial nuclei, generally accompanied by particle emission, and yielding a large amount of energy

gene: DNA sequence on a chromosome, forming a unit of inherited information, serving to achieve a **phenotypic** character through production of one (or more) **protein**. It contains the sequence coding for this protein, and sequences that enable and regulate **expression** of this sequence

genome: set of all genes governing an organism

**genomics** (structural): the science of **genomes**, bringing together an ensemble of analytical methods ranging from genome mapping to identification of new **genes**, through investigation of their functions and **sequencing** of DNA molecules

**geosphere:** part of the Earth serving as supporting substrate for all living organisms, comprising the outermost layer of the lithosphere, the hydrosphere, and the atmosphere

## gigaflops: see flops

grain boundary: interface between elementary crystals (grains) making up a material

hydrodynamics: part of fluid mechanics concerned with flows of incompressible fluids, or fluids not highly compressible, and the forces and pressures arising in such flows, as well with investigation of **turbulence** 

**implicit** (method): numerical resolution method for which the *entire set of variables* in the model are taken to be unknown at time *t*. This type of method requires more complex calculations than a **semi-implicit method**, but remains stable even over large time spans *in silico* ("in silicon"): refers to research methods using computers as experimental instruments, by analogy with *in vivo* or *in vitro* methods

**isotopes:** forms of the same element with nuclei having the same number of **protons**, and different numbers of **neutrons**. For instance, the 235- and 238-isotopes of uranium each have the same number of protons (92), but 143 neutrons for the 235-isotope, and 146 for the 238-isotope

iteration: in mathematics, resolution method for an equation, proceeding by successive approximations

**ligand:** molecule or ion bound to the central atom in a **complex** compound

**macromolecule:** molecule with a mass greater than thousands of daltons (the dalton is approximately equal to the mass of a hydrogen atom, i.e.  $1.66 \cdot 10^{-27}$  kg). This the case for **proteins** and **nucleic acids** 

metabolism: ensemble of chemical processes carried out in living cells

**metabolites:** organic compounds formed in the course of **metabolic** (synthesis or degradation) processes or contributing to them

**metabolomics:** simultaneous, comparative analysis of a large number of cell **metabolites** (small organic molecules), previously separated out

**mutation:** transmissible alteration of genetic inheritance, arising from the modification of a **nucleotide sequence** in **DNA** 

**nanometer** or **nanometric:** of a dimension of the order of a **nanometer** (10<sup>-9</sup> m), as certain **nanostructures** (e.g. **nanowires**)

**neutron:** elementary, electrically neutral particle, with a mass of  $1.675 \cdot 10^{-27}$  kg. The nature of this **nucleon** was discovered in 1932 by British physicist James Chadwick. Neutrons are the constituents, together with **protons**, of atomic nuclei

**neutronics:** study of the movement of **neutrons** in **fissile** and non-fissile materials, and the reactions they induce in matter, in particular inside nuclear reactors

Newtonian mechanics: the foundation of classical mechanics, this features three laws: 1. no change in the state of motion can occur without the action of some *force*; 2. the force exerted on a body is equal to the body's *mass* multiplied by its *acceleration*; 3. to every *action*, there is an associated *reaction*, that is equal and oppositely directed

**NMR (nuclear magnetic resonance):** principle of this method is based on the properties that certain atomic nuclei exhibit when placed in a strong magnetic field. They can then interact with radio waves to emit signals (spectra or images), allowing identification of the structure of the compounds present

**nucleic acids:** deoxyribonucleic acid (DNA) and ribonucleic acid (RNA). **DNA** is the molecular support for genetic information (genes). **RNA** is involved in the replication of the information in DNA. Messenger RNA, in particular, specifies the **amino-acid sequence** for a **protein** 

**nucleons:** constituent particles of the atom's nucleus, namely **protons** and **neutrons**, bound together by *strong interaction*, ensuring cohesiveness of the nucleus

# GLOSSARY

**nucleotide:** compound containing a **base** (purine or pyrimidine), a sugar and a phosphate group. **Purines** (adenine and guanine) and **pyrimidines** (cytosine and thymine) are two categories of cyclic compounds containing nitrogen

**nuclide:** nucleus species, characterized by its number of **protons** *Z*, number of **neutrons** *N*, and mass number *A*, equal to the sum of the number of protons and number of neutrons (A = Z + N)

**phase diagrams:** derived from the general laws of thermodynamics, these make it possible to know the composition, in terms of the various phases present, for a given alloy, as a function of temperature and concentrations in constituent elements

phenotype: set of all observable characters of an individual

**plasma:** medium made up of atoms in varying degrees of ionization, free electrons and photons

polymer: macromolecule consisting of the repetition of the same structural pattern, known as a monomer

**ppm:** part per million (ppb = part per billion)

**precipitate:** phase forming within a solution, with a concentration or crystalline structure different from that of the solution, when concentration exceeds the solubility limit

**primary** (in a thermonuclear device): nuclear **fission** warhead, conditioned by means of a chemical explosive, serving to yield the energy required for **fusion** of the (light-element) atoms in the thermonuclear stage

protein: macromolecule having the form of a long chain, comprising a sequence of amino acids

**proteomics:** discipline concerned with the translation, in given conditions, of **genes** into **proteins**, starting from the transcription in messenger **RNAs** 

**proton:** discovered in 1911 by British physicist Sir Ernest Rutherford, this **nucleon** carries a positive electric charge precisely equal and opposite to that of the electron. Its mass is equal to  $1.673 \cdot 10^{-27}$  kg

## purines; pyrimidines: see bases

**PWR (pressurized-water reactor):** the main family of common- (light-) water reactors. This type of reactor uses as coolant and moderator water that is kept liquid inside the core by maintaining appropriate pressure under normal operating conditions

**quantum:** (adj.) pertaining to the theory developed from Planck's quantum principle (exchanges of energy between matter and radiation may only occur in discrete packets) and Heisenberg's uncertainty principle, whereby simultaneous, accurate determination of both a particle's position and its velocity is not possible

### quantum mechanics: see quantum

**radioactivity:** property, exhibited by certain natural or artificial elements, of spontaneously emitting **alpha** particles (helium nuclei), **beta** particles (positrons [beta+ emission]) or electrons [beta- emission]), or **gamma** radiation (high-energy photons). More generally, this term refers to the emission of radiation concomitant with disintegration of an unstable element, or **fission** 

radioelement: element all isotopes of which are radioactive

radionuclide: radioactive isotope – sometimes also known as a radioisotope – of an element **reactivity:** in a **neutron**-multiplying environment, relative deviation, from the norm of 1, of the *effective multiplication factor*, this being the ratio, for a given time interval and for an environment of given composition and geometry, of the number of neutrons generated through **fission**, over the number of neutrons taken out

**relaxation:** return of a system, from a high-energy state (known as an excited state), to a stable state of lower energy

**repression** (of a gene): action of a **protein** binding to a specific **DNA** region, to inhibit transcription of an adjacent **gene** 

**residue:** in biochemistry, that part of a sugar, **amino acid** or **nucleotide** that is retained as part of a **polymer** chain, during the polymerization process

**resolution** (of a model): cell size, in terms of both time and space, selected in modeling

Schrödinger equation: fundamental equation of quantum mechanics, whose resolution allows determination of the system's energy, together with a function, the wave function, from which all of that system's properties may be derived. It was put forward by Erwin Schrödinger in 1926

**semi-implicit** (method): numerical resolution method, whereby *some variables* of the model are taken to be unknown at time *t*, whereas the others are held to be known (with the values for the preceding point in time) while the solution at time *t* is being sought. This type of method requires less computation than an **implicit** method, however it only remains stable if time intervals are kept sufficiently small

sequence: ordering of nucleotides in biological polymers (DNA, RNA, proteins). Sequencing is the determination of that order

**shockwave:** a discontinuity in the state of matter (pressure, temperature, density) propagating through a sample. It is usually caused by a perturbation

**site: sequence** in a **polymer** exhibiting specific properties; thus, the **active site** of an **enzyme protein** conditions its function

solvent: substance having the ability to dissolve a body

stochastic: featuring one or more random variables

teraflops: see flops

thermalhydraulics: part of physics concerned with heat transfers and fluid mechanics

**transmutation:** transformation, by spontaneous or induced nuclear reaction, of an atomic nucleus into a different one. The outcome may be transformation into a different chemical element, or simply **isotopic** change of the original element

tritium: very heavy isotope of hydrogen (hydrogen-3)

turbulence: flow mode for a fluid, where over the average motion is superimposed a random agitated motion

valence: number of bonds an atom may form

X-rays: electromagnetic waves with wavelengths, falling between those of ultraviolet and gamma radiation, comparable to interatomic distances

yeast: unicellular microscopic fungus