

process then translates back well to larger scale.

It is another object of the invention to identify potential issues with a process in silico prior to deployment on hardware, and to find process alternatives which overcome these issues.

The achievement of these objects in accordance with the invention is set out in the independent claims. Further developments of the invention are the subject matter of the dependent claims.

According to an aspect, the present disclosure refers to a computer-implemented method of scaling a production process to produce a chemical, pharmaceutical and/or biotechnological product, the scaling being from a source scale to a target scale, wherein the production process is defined by a plurality of steps specified by one or more process parameters controlling an execution of the production process, the method comprising:

- retrieving:

- parameter evolution information that describes the time evolution of the process parameter(s);

- a plurality of recipe templates, wherein:

a recipe comprises the plurality of steps defining the production process, and

a recipe template is a recipe in which at least one of the process parameters specifying the plurality of steps is a parameter being variable and having no predetermined value at the outset;

- receiving:

- a source setup specification of a source setup to be used for executing the production process at the source scale, the source setup specification comprising the source scale value;

- a target setup specification of a target setup to be used for executing the production process at the target scale, the target setup specification comprising the target scale value;

- a source recipe defining the production process at the source scale;
- at least one acceptability function defining conditions for the values of the process parameter(s) at the source scale and/or at the target scale;
- simulating the execution of the production process at the source scale using the source
- 5 setup specification, the source recipe and the parameter evolution information;
- determining, from the simulation, one or more source trajectories for the process parameter(s), wherein a trajectory corresponds to a time-based profile of values recordable during the simulated execution of the production process;
- performing a target determination step comprising:
- 10 -- selecting a recipe template pertinent to the production process out of the plurality of recipe templates;
- providing an input value for the at least one variable parameter in the selected recipe template;
- simulating the execution of the production process at the target scale using the target
- 15 setup specification, the selected recipe template, the input value for the at least one variable parameter and the parameter evolution information;
- determining, from the simulation, one or more target trajectories for the process parameters;
- comparing the source trajectory(ies) and the target trajectory(ies);
- 20 -- computing, based on the comparison and on the at least one acceptability function, an acceptability score for the selected recipe template;
- computing an optimal value for the at least one variable parameter in the selected recipe template by optimising the acceptability score and/or computing an acceptable range for the at least one variable parameter, wherein values within the acceptable
- 25 range yield an acceptability score above a specific threshold;
- if there is at least another pertinent recipe template, repeating the target determination step for at least another pertinent recipe template;
- selecting at least one of the plurality of recipe templates and corresponding computed value(s) for variable parameter(s) as target recipe based on the acceptability scores
- 30 computed for one or more recipe templates.

According to another aspect, the present disclosure refers to a computer-implemented method of scaling a production process to produce a chemical, pharmaceutical and/or biotechnological product, the scaling being from a source scale to an intermediate target scale to a final target scale, wherein the production process is defined by a plurality of steps specified by one or more process parameters controlling an execution of the production process, the method comprising:

- retrieving:

-- parameter evolution information that describes the time evolution of the process parameter(s);

-- a plurality of recipe templates, wherein:

a recipe comprises the plurality of steps defining the production process, and

a recipe template is a recipe in which at least one of the process parameters specifying the plurality of steps is a parameter being variable and having no predetermined value at the outset;

- receiving:

-- a source setup specification of a source setup to be used for executing the production process at the source scale, the source setup specification comprising the source scale value;

-- an intermediate target setup specification of an intermediate target setup to be used for executing the production process at the intermediate target scale, the intermediate target setup specification comprising the intermediate target scale value;

-- a final target setup specification of a final target setup to be used for executing the production process at the final target scale, the final target setup specification comprising the final target scale value;

-- a source recipe defining the production process at the source scale;

-- at least one acceptability function defining conditions on the values of the process parameter(s) when the values are considered singularly at any one of the source scale, intermediate target scale and final target scale and/or when the values at any one scale are considered in relation to corresponding values at any another one or more scales;

- simulating the execution of the production process at the source scale using the source setup specification, the source recipe and the parameter evolution information;

- determining, from the simulation, one or more source trajectories for the process parameter(s), wherein a trajectory corresponds to a time-based profile of values recordable during the simulated execution of the production process;
- performing a target determination step comprising:
 - 5 -- selecting a recipe template pertinent to the production process out of the plurality of recipe templates;
 - providing a first input value for the at least one variable parameter in the selected recipe template;
 - providing a second input value for the at least one variable parameter in the selected
 - 10 recipe template;
 - simulating the execution of the production process at the intermediate target scale using the intermediate target setup specification, the selected recipe template, the first input value for the at least one variable parameter and the parameter evolution information;
 - 15 -- determining, from the simulation, one or more intermediate target trajectories for the process parameters;
 - simulating the execution of the production process at the final target scale using the final target setup specification, the selected recipe template, the second input value for the at least one variable parameter and the parameter evolution information;
 - 20 -- determining, from the simulation, one or more final target trajectories for the process parameters;
 - making a first, a second and a third pairwise comparison between any two of the source trajectory(ies), the intermediate target trajectory(ies) and the final target trajectory(ies), and making a three-wise comparison among the source trajectory(ies),
 - 25 the intermediate target trajectory(ies) and the final target trajectory(ies);
 - computing an acceptability score based on at least two comparisons and on the at least one acceptability function;
 - computing a first optimal value and a second optimal value for the at least one variable parameter by optimising the acceptability score and/or
 - 30 computing a first acceptable range and a second acceptable range for the at least one variable parameter, wherein values within the first acceptable range and values within the second acceptable range yield an acceptability score above a specific threshold;

- if there is at least another pertinent recipe template, repeating the target determination step for at least another pertinent recipe template;
- selecting at least one of the plurality of recipe templates and corresponding computed value(s) for variable parameter(s) as target recipe based on the acceptability scores computed for one or more recipe templates.

According to another aspect, the present disclosure refers to a computer-implemented method of scaling a state of a production equipment for a production process to produce a chemical, pharmaceutical and/or biotechnological product, the scaling being from a source scale to a target scale, wherein the state is defined by a set of state parameters describing a condition and/or a behaviour of the production equipment, the method comprising:

- retrieving mapping information that describes how the state parameters relate to a set of derived parameters;

- receiving:

- a source setup specification of a source setup used for executing the production process at the source scale, the source setup specification comprising the source scale value;

- a target setup specification of a target setup used for executing the production process at the target scale, the target setup specification comprising the target scale value;

- a first set of state parameters at the source scale;

- a second set of state parameters at the target scale, wherein at least one of the state parameters at the target scale is a parameter being variable and having no predetermined value at the outset;

- at least one acceptability function defining conditions on the values of the state parameter(s) and/or the values of the derived parameter(s) at the source scale and/or at the target scale;

- calculating a first set of derived parameters at the source scale using the first set of state parameters, the source setup specification and the mapping information;

- providing an input value for the at least one variable parameter in the second set of state parameters;

- calculating a second set of derived parameters at the target scale using the second set of state parameters, the input value, the target setup specification and the mapping information;

- comparing the first set of state parameters with the second set of state parameters and/or comparing the first set of derived parameters and the second set of derived parameters;

- computing, based on the comparison and on the at least one acceptability function, an acceptability score for the second set of state parameters;

- computing an optimal value for the at least one variable parameter by optimising the acceptability score and/or computing an acceptable range for the at least one variable parameter, wherein values within the acceptable range yield an acceptability score above a specific threshold.

According to another aspect, the present disclosure refers to a computer-implemented method of scaling a state of a production equipment for a production process to produce a chemical, pharmaceutical and/or biotechnological product, the scaling being from a source scale to an intermediate target scale to a final target scale, wherein the state is defined by a set of state parameters describing a condition and/or a behaviour of the production equipment, the method comprising:

- retrieving mapping information that describes how the state parameters relate to a set of derived parameters;

- receiving:

-- a source setup specification of a source setup used for executing the production process at the source scale, the source setup specification comprising the source scale value;

an intermediate target setup specification of an intermediate target setup to be used for executing the production process at the intermediate target scale, the intermediate target setup specification comprising the intermediate target scale value;

-- a final target setup specification of a final target setup used for executing the production process at the final target scale, the final target setup specification comprising the final target scale value;

-- a first set of state parameters at the source scale;

- a second set of state parameters at the intermediate target scale, wherein at least one of the state parameters at the intermediate target scale is a first parameter being variable and having no predetermined value at the outset;
 - a third set of state parameters at the final target scale, wherein at least one of the
- 5 state parameters at the final target scale is a second parameter being variable and having no predetermined value at the outset;
- at least one acceptability function defining conditions on the values of the state parameter(s) and/or the values of the derived parameter(s) at the source scale and/or at the intermediate target scale and/or at the final target scale;
- 10 - calculating a first set of derived parameters at the source scale using the first set of state parameters, the source setup specification and the mapping information;
- providing a first input value for the at least one first variable parameter in the second set of state parameters;
 - calculating a second set of derived parameters at the intermediate target scale using
- 15 the second set of state parameters, the first input value, the intermediate target setup specification and the mapping information;
- providing a second input value for the at least one second variable parameter in the third set of state parameters;
 - calculating a third set of derived parameters at the final target scale using the third set
- 20 of state parameters, the second input value, the final target setup specification and the mapping information;
- making a plurality of pairwise comparisons within all pairs of any two of the first, second and third set of state parameters and/or within all pairs of any two of the first, second and third set of derived parameters, and making at least one three-wise
- 25 comparison among the first, second and third set of state parameters and/or among the first, second and third set of derived parameters;
- computing an acceptability score based on at least two comparisons and on the at least one acceptability function;
 - computing a first optimal value for the at least one first variable parameter and a
- 30 second optimal value for the at least one second variable parameter by optimising the acceptability score and/or

computing a first acceptable range for the at least one first variable parameter and a second acceptable range for the at least one second variable parameter, wherein values within the first acceptable range and values within the second acceptable range yield an acceptability score above a specific threshold.

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According to another aspect, the present disclosure refers to a computer program product comprising computer-readable instructions, which, when loaded and executed on a computer system, cause the computer system to perform operations according to the method of any one of the preceding aspects.

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According to another aspect, the present disclosure refers to a computer system operable to scale a production process to produce a chemical, pharmaceutical and/or biotechnological product from a source scale to a target scale, wherein the production process is defined by a plurality of steps specified by one or more process parameters controlling an execution of the production process, the computer system comprising:

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- a retrieving module configured to retrieve:
 - parameter evolution information that describes the time evolution of the process parameter(s);

- a plurality of recipe templates, wherein:

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- a recipe comprises the plurality of steps defining the production process, and
 - a recipe template is a recipe in which at least one of the process parameters specifying the plurality of steps is a parameter being variable and having no predetermined value at the outset;

- a receiving module configured to receive:

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- a source setup specification of a source setup to be used for executing the production process at the source scale, the source setup specification comprising the source scale value;

- a target setup specification of a target setup to be used for executing the production process at the target scale, the target setup specification comprising the target scale value;

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- a source recipe defining the production process at the source scale;

- at least one acceptability function defining conditions for the values of the process parameter(s) at the source scale and/or at the target scale; and
- a computing module configured to:
 - simulate the execution of the production process at the source scale using the source setup specification, the source recipe and the parameter evolution information;
 - determine, from the simulation, one or more source trajectories for the process parameter(s), wherein a trajectory corresponds to a time-based profile of values recordable during the simulated execution of the production process;
 - perform a target determination step comprising:
 - selecting a recipe template pertinent to the production process out of the plurality of recipe templates;
 - providing an input value for the at least one variable parameter in the selected recipe template;
 - simulating the execution of the production process at the target scale using the target setup specification, the selected recipe template, the input value for the at least one variable parameter and the parameter evolution information;
 - determining, from the simulation, one or more target trajectories for the process parameters;
 - comparing the source trajectory(ies) and the target trajectory(ies);
 - computing, based on the comparison and on the at least one acceptability function, an acceptability score for the selected recipe template;
 - computing an optimal value for the at least one variable parameter in the selected recipe template by optimising the acceptability score and/or computing an acceptable range for the at least one variable parameter, wherein values within the acceptable range yield an acceptability score above a specific threshold;
 - if there is at least another pertinent recipe template, repeat the target determination step for at least another pertinent recipe template;
 - select at least one of the plurality of recipe templates and corresponding computed value(s) for variable parameter(s) as target recipe based on the acceptability scores computed for one or more recipe templates.

According to one example, a computer-implemented method of scaling a production process to produce a chemical, pharmaceutical and/or biotechnological product is provided.

- 5 Examples of processes according to the present application are industrial processes, particularly biopharmaceutical processes. Other examples include research and development processes or scientific research.

10 Examples of inputs or ingredients for a production process according to the present application may include biological material, i.e. materials comprising a biological system, such as cells, cell components, cell products, and other molecules, as well as materials derived from a biological system, such as proteins, antibodies and growth factors. Further ingredients may include chemical compounds and various substrates.

- 15 Examples of inputs may include gasses and liquids. Gasses are any or all of air, oxygen, nitrogen, oxygen-enriched air and carbon dioxide. Liquids are typically:
- media (nutrient mix in buffer e.g. glucose + amino acids + salts + water)
 - inoculum (organism at relatively high density in media)
 - base (used to modulate pH e.g. ammonium hydroxide solution)
 - 20 - acid (used to modulate pH e.g. HCl solution)
 - nutrient feed (high concentration nutrient mix in buffer)
 - inducer (modulates behaviour of organism).