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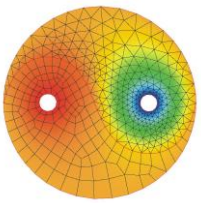

FRAMEWORK FOR FAST SIMULATIONS OF MATERIAL SCIENCE PHENOMENA WITH CAHN-HILLIARD EQUATIONS

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Abstract

This paper presents the framework for executing Cahn-Hilliard simulations through a web interface which is based on a popular continuous integration tool called Jenkins. This setup allows launching computations from any machine, in the client mode, and without the need to sustain a connection to the computational environment. It also isolates the researcher from the complexity of the underlying infrastructure and reduces the number of steps necessary to perform the simulations. Moreover, the results of the computations are automatically post-processed and stored upon job completion for future retrieval in the form of raw data, a sequence of bitmaps, as well as a video sequence illustrating changes in the material structure over time. The Cahn-Hilliard equations are parameterized with mobility and chemical potential function, allowing for several numerical applications. The discretization is performed with Isogeometric finite element method, and it is parameterized with the number of time steps, the time step size, the mesh size, and the order of the B-spline basis functions using for the approximation of the solution. The interface is linked with the alternating direction semi-implicit solver, resulting in a linear computational cost of the simulation.

Key words: Cahn-Hilliard equations, Material science simulations, Interface

1. INTRODUCTION

In this paper, we present a general framework for executing Cahn-Hilliard simulation through a web interface. The Cahn-Hilliard equations have several applications in material science, including the gamma to alpha transformation in C-MN steel, as described by Mecozzi et al. (2005). We focus on a general setup for the phase-separation modeling with the Cahn-Hilliard equations with the parameters following Gomez et al. (2008), and Elliot (1989). The general conclusions concerning the computational costs remain valid if we switch to metal forming related simulations. These simulations will require an update of the formulas for the mobility and chemical potential, following the ideas presented by Mecozzi et al. (2005). Our previous work concerned the application of iterative solvers to Cahn-Hilliard equations (Paszyński et al., 2018a), application of the refined Isogeometric analysis to C-H simulations (Paszyński et al., 2018b), as well as the development of the linearized time integration schemes (Schaefer et al., 2015).

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2. CAHN-HILLIARD EQUATIONS

The Cahn-Hilliard equation in its original form is:

$$\frac{du}{dt} = \nabla^{\circ}\left[M(u)\nabla\left(F(u) - \Delta u\right)\right] \quad in \quad \Omega \times [0;T] \quad (1)$$

defined over the square boundary $\Omega = [0,1]^2$, with periodic boundary conditions.

Let us make the following observations regarding equation (1):

- Equation (1) describes the concentration of one phase into another phase. The variable u has the value close to 0 if the second phase is dominant, and the value close to 1 when the first phase is dominant.
- The equation can model different phase-field phenomena, depending on the definition of the mobility function $M(u)$ and the chemical potential function $F(u)$. Exemplary definition of the functions for the phase-field simulations following Gomez et al. (2008) are

  $M(u) = u(1-u)$ and $F(u) = \frac{1}{2\theta}\log\left(\frac{u}{1-u}\right) + 1 - 2u$

  where θ is the ratio between the critical temperature, where two phases attain the same composition, and the absolute temperature. In order to make the phases separate, the θ parameter has to be greater than 1. In the exemplary simulation we use θ = 1.5, following Gomez et al. (2008). It is also possible to simulate a wide range of different physical phenomena, if the mobility and the chemical potential formulas are set to the corresponding values (Gomez et al., 2008).
- Equation (1) is the strong form of the Cahn-Hilliard problem. It contains fourth order derivatives (there is a divergence, a gradient and a Laplacian operator).
- The weak form can be obtained by the multiplication with test functions and integration by parts

$$\left(\frac{du}{dt}, v\right) = \left(\Delta u, \nabla\left[M(u)\nabla \mathrm{v}\right]\right) - \left(M(u)\nabla F(u), \nabla \mathrm{v}\right) \;\forall\; v \epsilon V \quad in \quad \Omega \times [0;T] \quad (2)$$

- where the brackets denote the L2 scalar product (integral of the multiplications of the components $(u,v) = \int uv dx$. Here, the Laplacian is multiplied by the gradient. Therefore, even after performing the integration by parts, there are second order weak derivatives in the corresponding weak form.
- This means that the standard finite elements with Lagrange polynomials are not applicable, since they are C^0 between finite elements and the second derivatives do not exist. One way to overcome this problem is to employ the Isogeometric Finite Element Method (Cottrel et al., 2009) with B-splines basis functions of order p, since they have the $C^{(p-1)}$ continuity between the finite elements. However, the cost of integration of the higher order B-splines basis functions is high (Woźniak, 2015). Furthermore, the cost of employing the direct solver algorithm is scaled by the factor of p^3 (Garcia et al., 2016). These two properties translate into the overall computational cost of the direct solver $O(N^{1.5}p^3)$, for two-dimensional simulations.

Following Gomez and Hughes (2011), it is possible to split the Cahn-Hilliard equations in their strong form into the system of second order equations by introducing the $\eta(u)$ term:

$$\begin{aligned} \frac{du}{dt} &= \nabla^{\circ}\left[M(u)\nabla\eta(u)\right] \quad in \quad \Omega \times [0;T] \\ \eta(u) &= F(u) - \Delta u \end{aligned} \quad (3)$$

We can make the following observations regarding equation (3):

- Eequation (3) describes the same physical process as equation (1), namely the concentration of one phase into another phase. The additional variable η has no physical meaning, it is an auxiliary scalar field that is defined as the potential function minus the Laplacian of the concentration.
- This time however, in the first and in the second sub-equations of equation (3), there are only the second order derivatives in the strong form, namely the scalar product of two gradients in the first one, and the Laplacian in the second one.
- The integration by parts leads to the system of weak problems given by:

$$\begin{aligned} \left(\frac{du}{dt}, v\right) &= \left(M(u)\nabla\eta(u), \nabla v\right) \forall\, v \epsilon V \; in \; \Omega \times [0;T] \\ \left(\frac{du}{dt}, v\right) &= \left(M(u)\nabla\eta(u), \nabla v\right) \forall\, v \epsilon V \; in \; \Omega \times [0;T] \end{aligned} \quad (4)$$

  where both the first and the second sub-problem is of the first order (it has only first order derivatives).
- This means that now we can utilize the Lagrange polynomials, that are C^0 between the finite elements. We can also use higher order B-splines ba-

sis functions which have the higher $C^{(p-1)}$ continuity, but this time it is not obligatory.
- Moreover, the system of equations (4) can be solved using the Alternating Direction solver (Puzyrev et al., 2019) that delivers a lower, linear $O(Np^3)$ computational cost.

Following the ideas of Gomez and Hughes (2011) and Puzyrev et al. (2019) we can solve the Cahn-Hilliard equations using the Alternating Direction solver (Paszyński et al., 2018a). In order to make the solver fully utilize the numerical properties of the underlying algorithm and considerably reduce the length of computations, a number of hardware-optimized numerical programming libraries, like Galois or Boost, had to be used. This in turn means that the process of running the simulations is different depending on the execution environment (the libraries need to be compiled and installed), which makes it difficult to reproduce across multiple environments. This work aims at automating this process, which makes the solver more available. Moreover, horizontal scaling of the execution environment is often required for long-running computations, like the ones described, to be able to perform a number of them in parallel, on multiple machines, often by many scientists. The setup described can be scaled up and down to any number of nodes.

3. INTERFACE

Responding to the problems above, we set up a web interface used to provide secure access to the underlying computational cluster in a transparent way. We utilized a set of tools popular in software engineering - Jenkins, for the web interface, and Ansible for achieving reproducible infrastructure, useful also for scaling the cluster size based on the number of concurrent tasks.

The Ansible scripts prepared as the part of the contribution of this paper are capable of replicating this computational environment onto any nodes (which meet certain criteria e.g. Debian-based operating system) by issuing one command. They set up a fully configured Jenkins cluster capable of running Cahn-Hilliard computational jobs. This setup allows launching the computations from any machine and without the need to sustain a connection to the computational environment. Moreover, the results of the computations are automatically post-processed and stored upon job completion for future retrieval in the form of raw data, a sequence of bitmaps, as well as a video sequence illustrating changes in the material structure over time. The jobs, including the scripts used to post-process data can be made a part of the solver code repository and be under version control. This in turn makes the solver a complete and coherent solution, which can be maintained, reviewed, automatically redeployed, tested and released. The solver is accessible through a web interface under the domain https://jenkins.a2s.agh.edu.pl/. Figure 1 shows the main page of this web interface.

There is one computational job available called cahn-hilliard. After clicking on the link, the user is redirected to the job details depicted in figure 2.

On the bottom left-hand side corner there is the list of historic tasks presented along with their execution date and the status. The new computational job can be triggered by pressing the build with parameters button, available in the top left-hand side corner. On the following screen, shown in figure 3, there input fields which contain the available configuration options. To run the computations described in the chapter 4.1 of the article by Gomez and Hughes (2011), we need to specify the mobility formula and the chemical potential formula. The first one should be set to: x(1-x), while the second to:

$$\frac{1}{2}\theta \log\left(\frac{x}{1-x}\right)+1-2x$$

We also need to provide the formula for the initial state. We do it by passing the contents of the function written in C programming language, which takes two arguments, x and y and returns the initial value in (x,y), to the corresponding text field. The default value corresponds to the plane with two circles situated in the top right (0.8,0.8) and the bottom left (0.2,0.2) corner of the plane, each 0.2 units in diameter. We may use any initial formulation we want, which may, but does not need to be (as this example demonstrates), a mathematical function. Then we select the size of the mesh (e.g. 50) and the time step delta (e.g. 0.000000001) as well as the time step count (e.g. 1000). Optionally, we can specify one or many e-mail addresses, in case we want to get a notification after the job is completed. After pressing the build button the user is redirected to the interactive computations log screen, shown in figure 4. The results of each computational task are made available under resource https://jenkins.a2s.agh.edu.pl/pub/<task_identifier>.

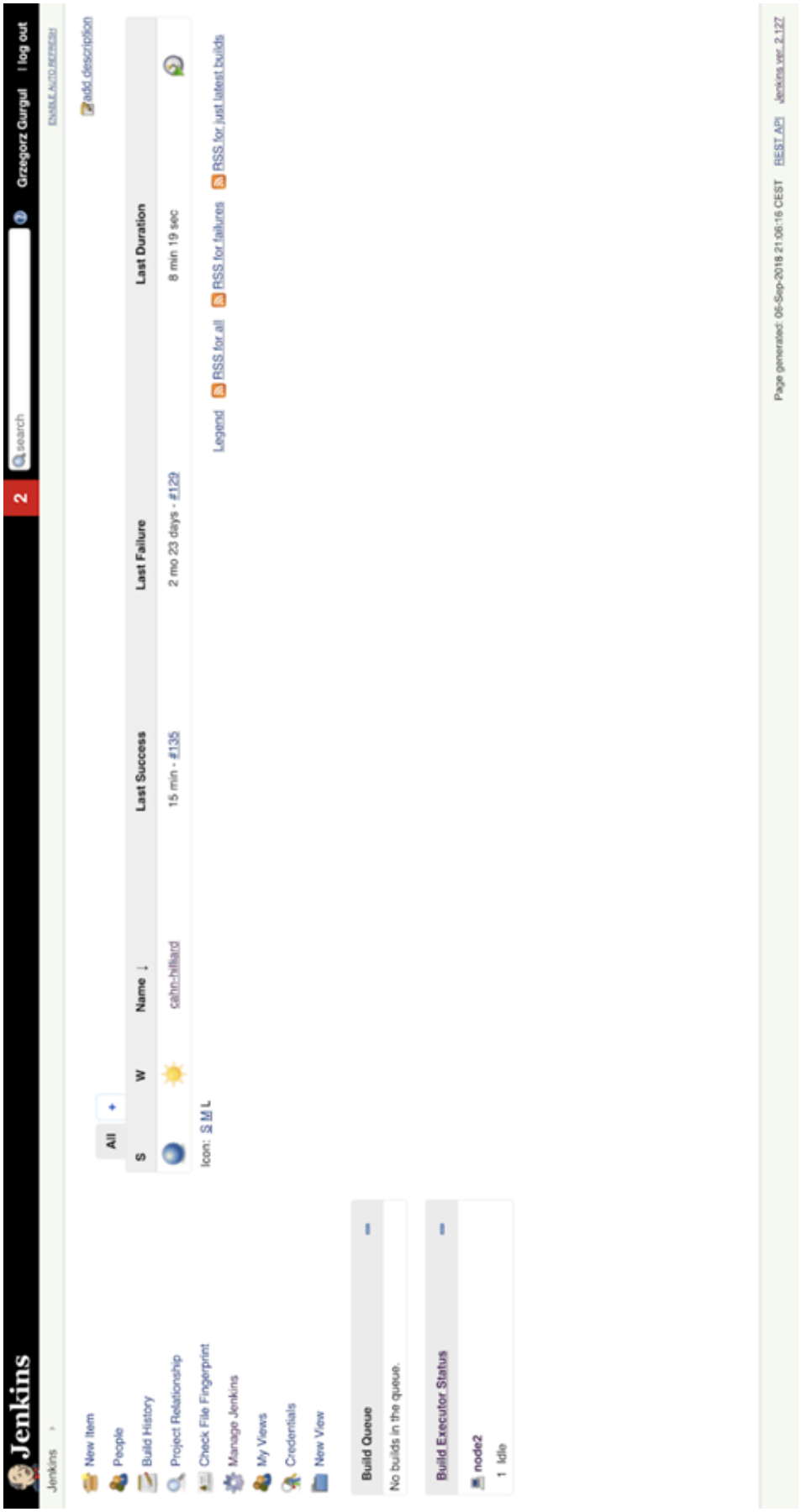


Fig. 1. *The main screen of the solver web interface.*

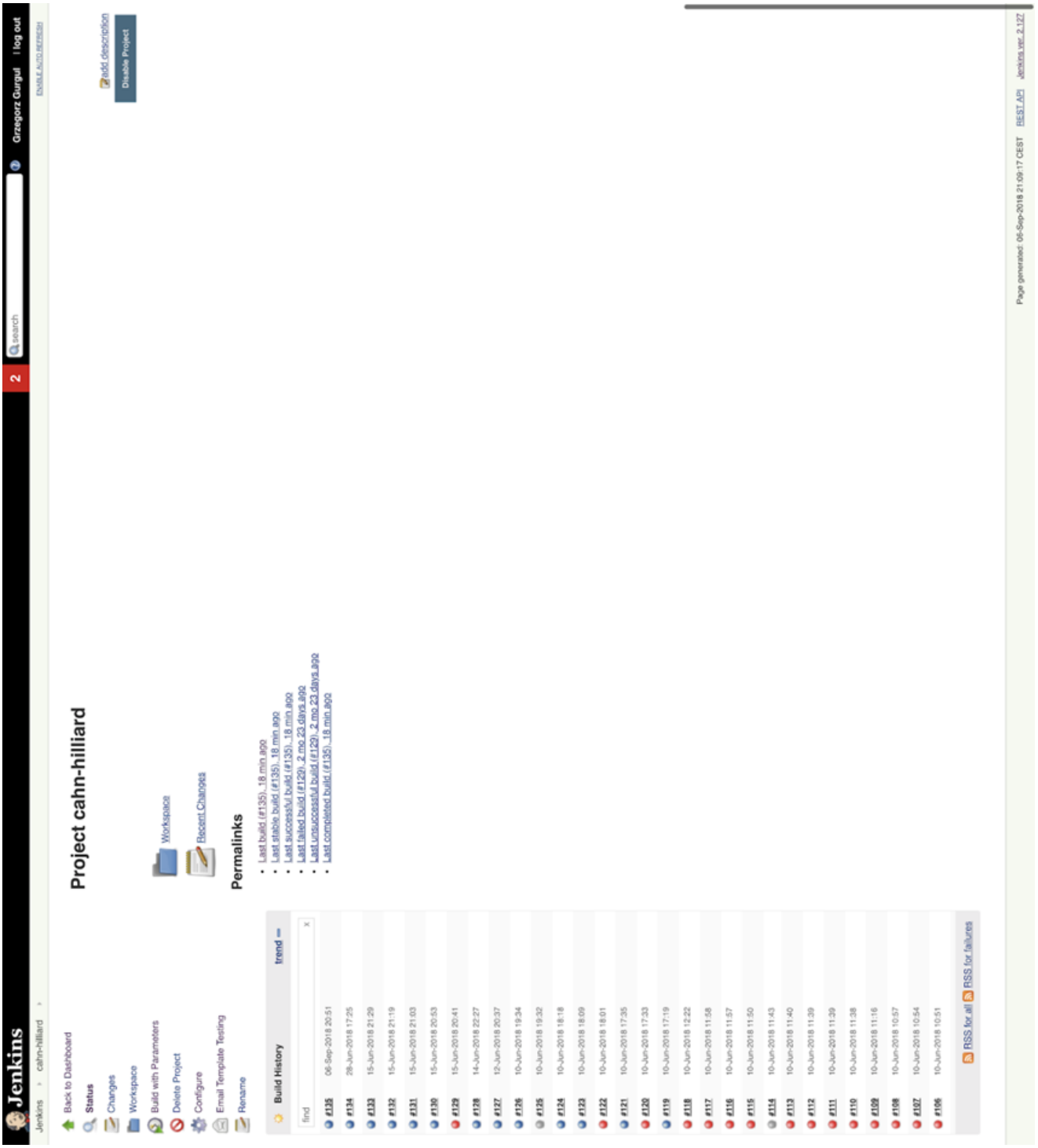
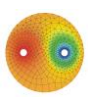


Fig. 2. *Cahn-Hilliard job details.*



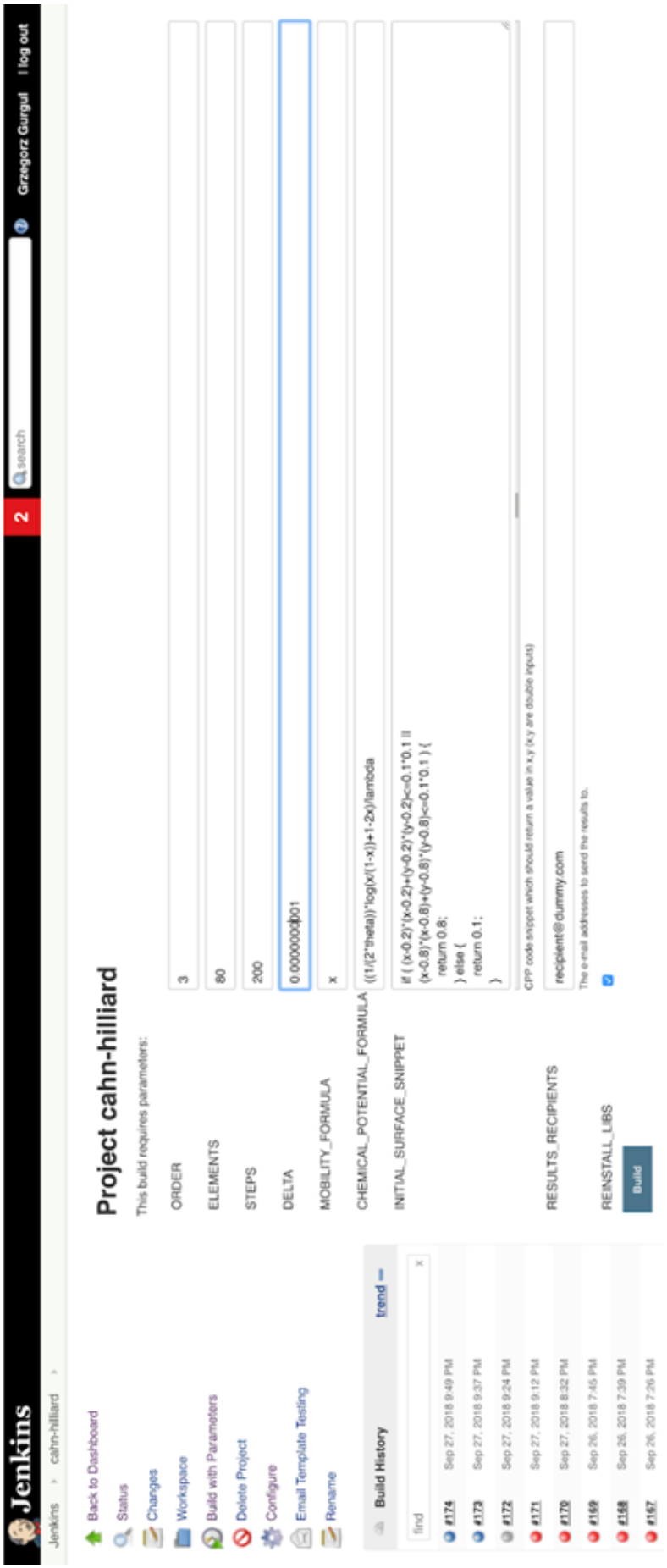


Fig. 3. *The computational task configuration screen.*

Fig. 4. *Computation log screen.*

The task identifier corresponds to the number of the job, for instance 135, in this example. The results are presented in a form of archives containing raw data, a set of pictures as well as a movie presenting change in the material structure over time.

4. NUMERICAL MODELLING

We validate the Cahn-Hilliard solver and the web interface it is accessible through using the example of the simulations of the physical phenomena of the process of the merging of two droplets, following Gomez and Hughes (2011). Figure 5 contains several frames of the visualization of the process, obtained by performing the steps described in chapter 3 of this paper.

The parameters used in this simulation are:

- Mesh size: 50×50
- Order of B-splines: Quadratic
- Number of time steps: 250,000
- Initial time step size: 10^{-10}
- Mobility function: $M(x) = 800x(1-x)$ (notice that interface takes variable x not u)
- Chemical potential: $F(c) = 4\gamma(c^3 - 6c^2 + 2c)$
- Initial configuration: two circles, one with the center in (0.35,0.35) and the radius 0.15, and one with the center (0.62,0.62) and the radius 0.2.

5. CONCLUSIONS

This paper presented a web-based interface to manage different numerical simulations of Cahn-Hilliard equation. The interface allows to provide different definitions of the mobility and chemical potenation functions, to make it possible to run different kind of simulations. It also allows for automatic compilation, linkage, execution and post-processing of the numerical results.

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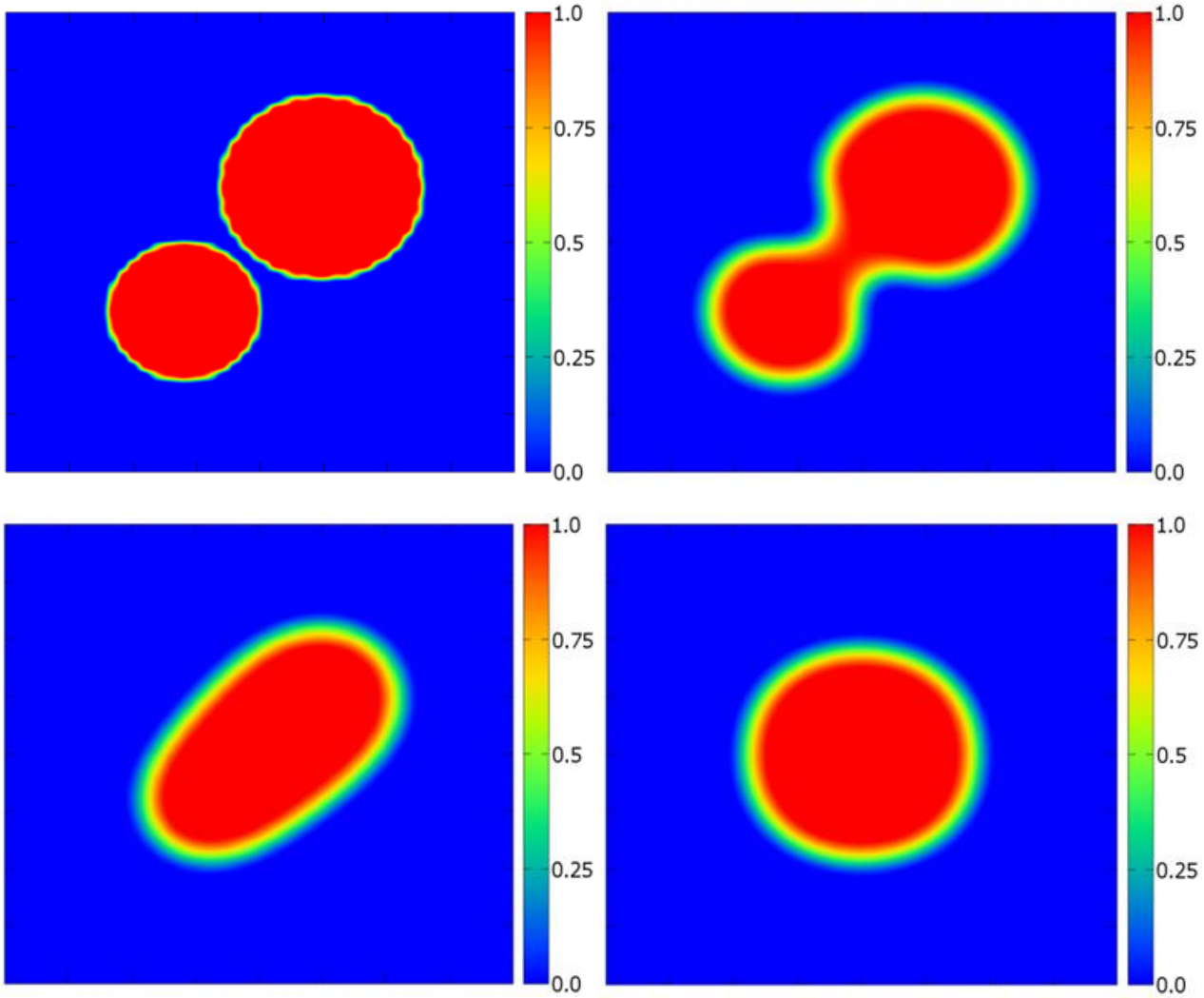

Fig. 5. *The process of merging of two droplets.*

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FRAMEWORK SŁUŻĄCY DO WYDAJNEJ SYMULACJI ZJAWISK FIZYCZNYCH W INŻYNIERII MATERIAŁOWEJ Z WYKORZYSTANIEM WZORÓW CAHNA-HILLIARDA

Streszczenie

W niniejszej pracy przedstawiamy framework służący do przeprowadzania symulacji opartych o wzory Cahna-Hilliarda poprzez wygodny interfejs webowy. Wykorzystujemy do tego popularne narzędzie służące do ciągłej integracji o nazwie Jenkins. Tego typu konfiguracja pozwala na uruchamianie obliczeń z dowolnej maszyny w trybie klienckim bez konieczności utrzymywania połączenia do środowiska obliczeniowego. Dzięki temu naukowiec wykonujący obliczenia jest odizolowany od skomplikowanej infrastruktury obliczeniowej, a uruchomienie symulacji wymaga mniejszej liczby czynności. Ponadto, wyniki symulacji są automatycznie przetwarzane i prezentowane w formie tabularycznej, sekwencji bitmap oraz filmu, który odzwierciedla zmiany zachodzące w strukturze badanego materiału w czasie. Równania Cahna-Hilliarda są parametryzowane poprzez funkcje mobilności i potencjału chemicznego, co pozwala na przeprowadzanie symulacji wybranych zjawisk dla wielu materiałów. Dyskretyzacja jest wykonywana z wykorzystaniem Izogeometrycznej Metody Elementów Skończonych i jest uzależniona od liczby i rozmiaru kroków czasowych, wielkości siatki oraz rzędu krzywych B-sklejanych, użytych do aproksymacji rozwiązania. Interfejs, o którym mowa, konfiguruje solwer zmienno-kierunkowy z dyskretyzacją czasową schematem wprost, co skutkuje liniowym kosztem obliczeniowym symulacji.

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