

Multi-Component Multiphase Compressible Hydrodynamics: Current State

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Abstract. The dynamic loading of multi-component materials disturbs them from equilibrium and generates relaxation processes in which components interact with each other exchanging momentum and energy (and mass if chemical reactions occur). The description of exchange processes through pair interactions allows considering the individual properties of interacting components (particle size, surface roughness, adhesion etc.). The paper discusses a new type of interaction, namely a cluster interaction which gives a new force tensor and new energy fluxes whose dependences on the characteristics of each component and on barycentric velocity are proposed and validated. The author introduces a concept of non-equilibrium kinetic energy for a component and proposes a new equation for volume concentrations which closes the system of conservation equations along with an equation of state for the i -th component, and does not impose additional restrictions on mixture properties. The model admits state and phase changes in each component.

INTRODUCTION

Pure materials are very few in nature. Mixtures are most often. If a small volume $d\theta$ contains several ($N > 1$) materials, each of the materials is called a component and the medium in the volume is called multi-component. Impacts on a multi-component medium lead to displacements of its components, to their mixing or separation, heating and deformation, phase transitions or changes in the state of aggregation (i.e., thixotropy), chemical reactions in the components and other changes.

The history of multicomponent models goes back to the middle of the XIX century but their theory is still to be completed. Necessary information is still being collected through study and application of particular models. In what all models are weak is the description of interactions between components. Two fundamental problems remain unsolved:

- Derivation of conservation laws for a mixture from the conservation laws for its components; and
- Closure of the system of equations for the i -th component.

Both have been challenging for science during several decades. Below are their solutions.

1. MULTICOMPONENT MODELS

All multicomponent models can be classified into diffusion models and multivelocity continua models in which the behavior of each component is defined by conservation laws for macro-scale quantities. This means that we have passed from micro- to macro-scale quantities and each i -th component is a continuum physically characterized by a pressure P_i , a temperature T_i , a density ρ_i , a specific internal energy E_i , a velocity \bar{U}_i , an entropy S_i etc. Thermodynamic parameters of the i -th component are related through an equation of state.

Consider a small volume $d\theta$ containing a mixture of N component of a mass dM . Divide dM and $d\theta$ between all components:

$$dM = \sum_{i=1}^N dM_i, \quad d\theta = \sum_{i=1}^N d\theta_i. \quad (1)$$

The ratios

$$\eta_i = \frac{dM_i}{dM}, \quad \alpha_i = \frac{d\theta_i}{d\theta} \quad (2)$$

are called [1-5] mass and volume concentrations of the i -th component. Density is defined as a mass of material per unit volume. Therefore

$$\rho_i = \frac{dM_i}{d\theta_i} \quad \text{and} \quad \rho = \frac{dM}{d\theta}, \quad (3)$$

where ρ_i is the density of the i -th component and ρ is the density of the mixture. Assume that the mass dM_i is “smeared” over the entire volume $d\theta$. The quantity

$$\alpha_i \rho_i = \frac{dM_i}{d\theta} \quad (4)$$

is virtual and called a partial density of the i -th component. It follows from (2)-(4) that $\alpha_i \rho_i$ and ρ relate as

$$\alpha_i \rho_i = \eta_i \rho. \quad (5)$$

For the specific volume $V = 1/\rho$, the equation (5) takes the form

$$\alpha_i V = \eta_i V_i. \quad (6)$$

It follows from (1), (3) and (4) that the density of the mixture is a sum of the partial densities:

$$\rho = \sum_{i=1}^N \alpha_i \rho_i . \quad (7)$$

Each component is characterized by a momentum $\bar{U}_i dM_i$. The law of momentum conservation at a fixed time t gives

$$\bar{U} dM = \sum_{i=1}^N \bar{U}_i dM_i .$$

Replacing dM_i by $\eta_i dM$ with (2) and canceling dM give that the mixture velocity \bar{U} is a sum of the partial velocities $\eta_i \bar{U}_i$:

$$\bar{U} = \sum_{i=1}^N \eta_i \bar{U}_i . \quad (8)$$

It follows from (5) and (8) that the specific momentum $\rho \bar{U}$ of the mixture is a sum of specific momenta for components:

$$\rho \bar{U} = \sum_{i=1}^N \alpha_i \rho_i \bar{U}_i . \quad (9)$$

The velocity \bar{U} defined by (8) is called the barycentric velocity [1, 2].

The specific internal energy E is energy per unit mass. The law of internal energy conservation at a fixed time gives

$$E dM = \sum_{i=1}^N E_i dM_i .$$

Dividing by dM and using (2) give that the specific energy of a mixture is a sum of the partial specific internal energies for components:

$$E = \sum_{i=1}^N \eta_i E_i . \quad (10)$$

Similar manipulations with the specific energy give the following equation for the total specific energy ε :

$$\varepsilon = \sum_{i=1}^N \eta_i \varepsilon_i . \quad (11)$$

Using (6), rewrite (10) and (11) in the forms

$$\rho E = \sum_{i=1}^N \alpha_i \rho_i E_i \quad \text{and} \quad \rho \varepsilon = \sum_{i=1}^N \alpha_i \rho_i \varepsilon_i . \quad (12)$$

$E(V,S)$ and $E_i(V_i,S_i)$ are thermodynamic potentials and their differentials are

$$dE = \left(\frac{\partial E}{\partial V} \right)_S dV + \left(\frac{\partial E}{\partial S} \right)_V dS \quad \text{and} \quad dE_i = \left(\frac{\partial E_i}{\partial V_i} \right)_{S_i} dV_i + \left(\frac{\partial E_i}{\partial S_i} \right)_{V_i} dS_i . \quad (13)$$

For $S = \text{const}$ and $S_i = \text{const}$, differentiate (6) and (10) with respect to the thermodynamic variables V, S and V_i, S_i bearing in mind that η_i and α_i are independent of V, S and V_i, S_i . We obtain two equations

$$\left(\frac{\partial E}{\partial V}\right)_S dV = \sum_{i=1}^N \left(\frac{\partial E_i}{\partial V_i}\right)_{S_i} \eta_i d_i V_i \quad \text{and} \quad \alpha_i dV = \eta_i d_i V_i$$

which give

$$\left(\frac{\partial E}{\partial V}\right)_S = \sum_{i=1}^N \left(\frac{\partial E_i}{\partial V_i}\right)_{S_i} \alpha_i. \quad (14)$$

Since

$$P = -\left(\frac{\partial E}{\partial V}\right)_S \quad \text{and} \quad P_i = -\left(\frac{\partial E_i}{\partial V_i}\right)_{S_i},$$

the equation (14) means that the total pressure is a sum of the partial pressures:

$$P = \sum_{i=1}^N \alpha_i P_i. \quad (15)$$

This is a general equation. For the case of ideal gases with identical temperatures $T_i = T$, it was proved by Dalton and was called Dalton law.

$P_i, \rho_i, E_i, T_i, \bar{U}_i$ and others are macro-scale quantities of the i -th component which describe it as a continuum. However, each component is a structural element of the mixture. So, these parameters are meso-scale quantities of the mixture. The macro-scale quantities characterizing the behavior of the mixture are derived from the meso-scale quantities with the equations (7), (8), (10), (11), and (15).

2. COMPONENT INTERACTIONS

A multicomponent medium may not be in equilibrium. Mixture equilibrium conditions are

$$P_i = P_j, \quad T_i = T_j, \quad \bar{U}_i = \bar{U}_j.$$

If at least one of them is not satisfied, the mixture is not in equilibrium; it tries to attain equilibrium through a number of relation processes in which mixture components exchange momentum and energy.

For a long time, multicomponent models have considered only pair interactions in which the i -th and j -th components interact independently of all others [1-4]. If $\bar{U}_i \neq \bar{U}_j$, the exchange of their momenta is most often defined by the vector

$$\bar{R}_{ji} = a_{ij} (\bar{U}_j - \bar{U}_i) / \tau_{ij}^U.$$

The functions a_{ij} and τ_{ij}^U depend on the degree of heterogeneity, on the properties of the i -th and j -th components, on the size of their particles, on sound velocity,

compressibility, equations of state for the components, on their states of aggregation, adhesion and other properties in such a way as to satisfy Onsager reciprocity condition

$$a_{ij} = a_{ji}, \quad \tau_{ij}^U = \tau_{ji}^U,$$

due to which \bar{R} satisfies the condition

$$\bar{R}_{ij} = -\bar{R}_{ji}.$$

Specific forms for the dependencies are established from the conditions of each particular problem. They are often validated using a unit cell of two components. The order of the indices ij indicates that the j -th component acts on the i -th one. The action of all N components (i.e., the mixture) on the i -th one is accomplished through summation with respect to j

$$\bar{R}_{Si} = \sum_{j=1}^N \alpha_j \bar{R}_{ji}. \quad (16)$$

From (16), \bar{R}_S acting on the mixture from all components vanishes:

$$\bar{R}_S = \sum_{j=1}^N \sum_{i=1}^N \alpha_i \alpha_j \bar{R}_{ij} = 0. \quad (17)$$

Similar reasoning applies to a scalar function Φ_{ij} which describes energy exchange between the i -th and j -th components. As a rule [4], the function is taken in the form

$$\Phi_{ji} = \frac{b_{ji}}{\tau_{ji}^P} (P_j - P_i) + \frac{c_{ji}}{\tau_{ji}^T} (T_j - T_i), \quad (18)$$

where

$$b_{ij} = b_{ji}, \quad c_{ij} = c_{ji}, \quad \tau_{ij}^P = \tau_{ji}^P, \quad \tau_{ij}^T = \tau_{ji}^T, \quad \Phi_{ji} = -\Phi_{ij}.$$

The flux of energy to the i -th component from all others results from summation:

$$\Phi_{Si} = \sum_{j=1}^N \alpha_j \Phi_{ji}.$$

The energy flux acting on the mixture from all components is zero:

$$\Phi_S = \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j \Phi_{ij} = 0. \quad (19)$$

The equations (17) and (19) are fundamental to the pair interaction models.

With the equations (7), (8), (10), (11) and (15) for the macro-scale quantities ρ , \bar{U} , E , ε and P , we can introduce a new type of interaction in which each i -th component interacts with the mixture. Call it a **cluster** interaction. In this interaction, momentum and energy changes in the i -th component are controlled by the parameters P , ρ , E , \bar{U} , and T for the mixture and by the parameters P_i , ρ_i , E_i , \bar{U}_i , and T_i for the i -th component. To express the cluster interaction, introduce a force tensor and an energy

flux. Let F_{Si} stand for the tensor of forces to the i -th component from the mixture and \bar{Q}_{Si} for the energy flux. They satisfy the cluster interaction conditions

$$F_S = \sum_{i=1}^N \alpha_i F_{iS} = -\sum_{i=1}^N \alpha_i F_{Si}, \quad \bar{Q}_S = \sum_{i=1}^N \alpha_i \bar{Q}_{iS} = -\sum_{i=1}^N \alpha_i \bar{Q}_{Si}. \quad (20)$$

3. CONSERVATION LAWS FOR COMPONENTS

Write the conservation laws for mass, momentum and energy as

$$\frac{\partial}{\partial t}(\alpha_i \rho_i) + \nabla(\alpha_i \rho_i \bar{U}_i) = 0, \quad (21)$$

$$\frac{\partial}{\partial t}(\alpha_i \rho_i \bar{U}_i) + \nabla \alpha_i P_i + \sum_{k=1}^3 \frac{\partial}{\partial x_k}(\alpha_i \rho_i \bar{U}_i U_{ki} + \alpha_i \bar{F}_{kSi}) - \alpha_i \bar{R}_{Si} = 0, \quad (22)$$

$$\frac{\partial}{\partial t}(\alpha_i \rho_i \varepsilon_i) + \nabla(\alpha_i \bar{U}_i (P_i + \rho_i \varepsilon_i)) + \sum_{k=1}^3 \frac{\partial}{\partial x_k}(\alpha_i \bar{F}_{kSi} \bar{U}_i) + \nabla \alpha_i \bar{Q}_{Si} - \alpha_i \Phi_{Si} - \alpha_i A_{Si} = 0. \quad (23)$$

Here A_{Si} is the work of the vector \bar{R}_{Si} defined as

$$A_{Si} = 0.5 \sum_{j=1}^N \alpha_j \bar{R}_{ji} (\bar{U}_i + \bar{U}_j).$$

Add to the equations (21)-(23) an equation of state in the form

$$P_i = P_i(\rho_i, E_i), \quad T_i = T_i(\rho_i, E_i)$$

and an equation for ε_i in terms of E_i and $0.5\bar{U}_i^2$:

$$\varepsilon_i = E_i + 0.5\bar{U}_i^2. \quad (24)$$

Compared with [1-3], these equations contain several new quantities, namely a vector \bar{F}_{kSi} created by elements of the k -th line of F_{Si} , a vector \bar{Q}_{Si} , and a scalar A_{Si} .

The macro-scale quantities P , ρ , E , \bar{U} , ε , and T characterize a continuum (a mixture). Write mass, momentum and energy conservation laws for the mixture with the cluster interaction in the form

$$\frac{\partial \rho}{\partial t} + \nabla \rho \bar{U} = 0, \quad (25)$$

$$\frac{\partial}{\partial t}(\rho \bar{U}) + \bar{U} \nabla(\rho \bar{U}) + \rho(\bar{U} \nabla) \bar{U} + \nabla P + \sum_{k=1}^3 \frac{\partial}{\partial x_k} \bar{F}_{kS} = 0, \quad (26)$$

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \nabla \bar{U}(\rho \varepsilon) + \sum_{k=1}^3 \frac{\partial}{\partial x_k}(\bar{U} \bar{F}_{kS}) + \nabla \bar{Q}_S = 0. \quad (27)$$

\bar{F}_{ks} contains elements of the k -th line of \bar{F}_s defining the force to the mixture from all components. F_s and F_{si} , \bar{Q}_s and \bar{Q}_{si} are related through the cluster interaction condition (20).

4. FORCE TENSOR F_{Si}

Let $\delta\bar{U}_i = \bar{U}_i - \bar{U}$ be velocity oscillations round a mean \bar{U} . Substitute

$$\bar{U}_i = \bar{U} + \delta\bar{U}_i$$

in the momentum equation for the i -th component (22) and sum with respect to i . We obtain

$$\frac{\partial}{\partial t}(\rho\bar{U}) + \bar{U}\nabla(\rho\bar{U}) + \rho(\bar{U}\nabla)\bar{U} + \nabla P + \sum_{i=1}^N \sum_{k=1}^3 \frac{\partial}{\partial x_k}(\alpha_i(\bar{F}_{ksi} + \rho_i\delta\bar{U}_i\delta\bar{U}_{ki})) = 0. \quad (28)$$

The first four terms in this equation coincide with those in the equation (26). Equation (28) coincides with the equation (26) if

$$\sum_{i=1}^N \sum_{k=1}^3 \frac{\partial}{\partial x_k}(\alpha_i(2\bar{F}_{ksi} + \rho_i(\bar{U}_i - \bar{U})(U_{ki} - U_k))) = 0.$$

Zeroing each of the summands, integrating with respect to x_k , and requiring that $\bar{F}_{ksi} = 0$ at $\bar{U}_i = \bar{U}$ gives the following equation for \bar{F}_{ksi} :

$$\bar{F}_{ksi} = -0.5\rho_i(\bar{U} - \bar{U}_i)(U_k - U_{ki}). \quad (29)$$

5. ENERGY FLUX \bar{Q}_{Si}

The specific kinetic energy of velocity oscillations is

$$H_i = 0.5(\bar{U}_i - \bar{U})^2. \quad (30)$$

It follows from the conservation laws for each type of energy at $t = \text{const}$ that

$$\rho H = \sum_{i=1}^N \alpha_i \rho_i H_i. \quad (31)$$

Substituting (30) into (31) and using (7) and (9) yield

$$\rho H + 0.5\rho\bar{U}^2 = \sum_{i=1}^N 0.5\alpha_i \rho_i \bar{U}_i^2. \quad (32)$$

Using (12), express the mixture parameters $P\bar{U}$, $\rho\varepsilon$, $\rho\varepsilon\bar{U}$, \bar{Q}_s , \bar{F}_{ks} , and A_s in terms of partial quantities

$$P\bar{U} = \sum_{i=1}^N \alpha_i P_i \bar{U}_i + \sum_{i=1}^N \alpha_i P_i (\bar{U} - \bar{U}_i), \quad \rho \varepsilon \bar{U} = \sum_{i=1}^N \alpha_i \rho_i \varepsilon_i U_i + \sum_{i=1}^N \alpha_i \rho_i \varepsilon_i (\bar{U} - \bar{U}_i),$$

$$\bar{Q}_S = -\sum_{i=1}^N \alpha_i \bar{Q}_{Si}, \quad \bar{F}_{kS} = -\sum_{i=1}^N \alpha_i \bar{F}_{kSi}, \quad -\sum_{i=1}^N \alpha_i A_{Si} = 0, \quad -\sum_{i=1}^N \alpha_i \Phi_{Si} = 0$$

and substitute in (27). We obtain

$$\begin{aligned} & \sum_{i=1}^N \left[\frac{\partial}{\partial t} (\alpha_i \rho_i \varepsilon_i) + \nabla (\alpha_i \bar{U}_i (P_i + \rho_i \varepsilon_i)) + \right. \\ & \left. + \sum_{k=1}^3 \frac{\partial}{\partial x_k} (\alpha_i \bar{F}_{kSi} \bar{U}_i) + \nabla \alpha_i \bar{Q}_{Si} - \alpha_i \Phi_{Si} - \alpha_i A_{Si} + B_i \right] = 0, \end{aligned} \quad (33)$$

where

$$B_i = \nabla (\alpha_i (P_i + \rho_i \varepsilon_i) (\bar{U} - \bar{U}_i)) - 2 \nabla \alpha_i \bar{Q}_{Si} - \sum_{k=1}^3 \frac{\partial}{\partial x_k} (\alpha_i \bar{F}_{kSi} (\bar{U} + \bar{U}_i)).$$

Each i -th summand in (33) coincide with the energy equation (23) for the i -th component if $B_i = 0$. Using (24) and (29), rewrite it as

$$\nabla (\alpha_i ((\bar{U} - \bar{U}_i) (P_i + \rho_i E_i) - 2 \bar{Q}_{Si})) = 0. \quad (34)$$

Integrating (34) with respect to x_k and finding integration constants from the condition that $\bar{Q}_{Si} = 0$ at $\bar{U}_i = \bar{U}$ give the following expression for the energy flux:

$$\bar{Q}_{Si} = 0.5 (\bar{U} - \bar{U}_i) (P_i + \rho_i E_i). \quad (35)$$

With the equations (29) and (35) for \bar{F}_{kSi} and \bar{Q}_{Si} , the conservation laws (21)-(23) for the i -th component are invariant to Galilean transformation and have the property that the summation of conservation laws for components with respect to i gives corresponding conservation laws for the mixture. The first of the above two problems is thus resolved.

6. COROLLARIES TO CONSERVATION LAWS

Before we start to manipulate the conservation laws (21)-(23) and (25)-(27), consider components of the total specific energy ε . Multiply ε_i (24) by $\alpha_i \rho_i$ and sum with respect to i :

$$\sum_{i=1}^N \alpha_i \rho_i \varepsilon_i = \sum_{i=1}^N \alpha_i \rho_i E_i + \sum_{i=1}^N 0.5 \alpha_i \rho_i \bar{U}_i^2.$$

After substituting (12) and (32) in this equation and canceling ρ we obtain

$$\varepsilon = E + 0.5 \bar{U}^2 + H.$$

Thus the total specific energy of the mixture, ε , is the sum of the specific internal energy of the mixture, E , the specific kinetic energy of the mixture, $0.5\bar{U}^2$, and the specific non-equilibrium kinetic energy of the mixture, H (specific energy of velocity oscillations). As velocity relax, H goes into E .

Applying identical transformations to the conservation laws (21)-(23) for the i -th component and (25)-(27) for the mixture gives equations of motion, equations for the specific internal energy, and equations for specific entropy:

$$\begin{aligned}
& \alpha_i \rho_i \frac{d_i \bar{U}_i}{dt} + \nabla \alpha_i P_i + \sum_{k=1}^3 \frac{\partial}{\partial x_k} (\alpha_i \bar{F}_{kSi}) - \alpha_i \bar{R}_{Si} = 0, \\
& \alpha_i \rho_i \frac{d_i E_i}{dt} + \alpha_i \left(P_i \nabla \bar{U}_i + \sum_{k=1}^3 \bar{F}_{kSi} \frac{\partial \bar{U}_i}{\partial x_k} + \bar{R}_{Si} \bar{U}_i - A_{Si} - \Phi_{Si} \right) + \nabla \alpha_i \bar{Q}_{Si} = 0, \\
& \alpha_i \rho_i T_i \frac{d_i S_i}{dt} - P_i \frac{d_i \alpha_i}{dt} + \alpha_i \left(\sum_{k=1}^3 \bar{F}_{kSi} \frac{\partial \bar{U}_i}{\partial x_k} + \bar{R}_{Si} \bar{U}_i - A_{Si} - \Phi_{Si} \right) + \nabla \alpha_i \bar{Q}_{Si} = 0, \quad (36) \\
& \rho \frac{d\bar{U}}{dt} + \nabla P + \sum_{k=1}^3 \frac{\partial \bar{F}_{kS}}{\partial x_k} = 0, \\
& \rho \frac{dE}{dt} + \rho \frac{dH}{dt} + P \nabla \bar{U} + \sum_{k=1}^3 \bar{F}_{kS} \frac{\partial \bar{U}}{\partial x_k} + \nabla \bar{Q}_S = 0, \\
& \rho T \frac{dS}{dt} + \frac{\partial \rho H}{\partial t} + \nabla (\rho H \bar{U}) + \sum_{k=1}^3 \bar{F}_{kS} \frac{\partial \bar{U}}{\partial x_k} + \nabla \bar{Q}_S = 0. \quad (37)
\end{aligned}$$

For $V = \text{const}$ and $V_i = \text{const}$, and for η_i and α_i independent of thermodynamic quantities, the equations

$$dE = \sum_{i=1}^N \eta_i d_i E_i, \quad dE = \left(\frac{\partial E}{\partial S} \right)_V dS, \quad d_i E_i = \left(\frac{\partial E_i}{\partial S_i} \right)_{V_i} d_i S_i, \quad T = \left(\frac{\partial E}{\partial S} \right)_V, \quad T_i = \left(\frac{\partial E_i}{\partial S_i} \right)_{V_i}$$

give

$$TdS = \sum_{i=1}^N \eta_i T_i d_i S_i.$$

Using (6), the equation can be written as

$$\rho T dS = \sum_{i=1}^N \alpha_i \rho_i T_i d_i S_i.$$

Dividing by dt gives

$$\rho T \frac{dS}{dt} = \sum_{i=1}^N \alpha_i \rho_i T_i \frac{d_i S_i}{dt} \quad (38)$$

which expresses entropy production for the mixture as the sum of entropy productions for components.

Substituting (37) and (36) in (38) gives the equation for the volume concentration of the i -th component:

$$P_i \frac{d_i \alpha_i}{dt} + (\bar{U} - \bar{U}_i) \nabla \alpha_i P_i - 2 \nabla \alpha_i Q_{Si} = 0. \quad (39)$$

This equation closes the conservation laws for the i -th component. Thus the second problem is also resolved.

7. MODEL PROPERTIES

The new force F_{Si} (29) and energy flux \bar{Q}_{Si} (35) contain quantities with the subscript i which characterize components, or structural elements of a multicomponent medium and only two macro-scale quantities, namely density ρ and velocity \bar{U} of the mixture. The force F_{Si} and the flux \bar{Q}_{Si} are universal; they do not contain empiric constants and do not depend on component characteristics or properties which control relaxation times. This is the property in which the cluster interaction fundamentally differs from the pair one.

The force F_{Si} and the flux \bar{Q}_{Si} vanish as velocity equilibrium establishes. It follows from (39) that at $\bar{U}_i = \bar{U}$ the volume concentrations of components remain constant along trajectories.

Conservation laws for a multicomponent medium result from the summation of the laws for components. This property of the model is no more than an argument in its favor because the behavior of the i -th component can be described without these laws. Equations for the i -th component include the conservation laws (21)-(23), equations for A_{Si} , \bar{F}_{Si} , \bar{Q}_{Si} , \bar{R}_{Si} , Φ_{Si} and ε_i , the equation (39) for α_i , equations of state, and the equations (8) and (9) for ρ and U . So, the number of equations and the number of functions are identical in the full system of equations which is closed with no additional hypotheses specifying the mixture. The model presented makes it possible to describe concurrently a lot of phenomena in multicomponent media and even increase the accuracy of predictions for systems not yet studied experimentally.

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