様　式　C－１９、F－１９－１、Z－１９　（共通）

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研究課題名（和文）Understanding plasticity of metals through proving discrete-to-continuum limits of interacting particle systems

研究課題名（英文）Understanding plasticity of metals through proving discrete-to-continuum limits of interacting particle systems

研究代表者
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交付決定額（研究期間全体）：（直接経費）　　2,400,000円

研究成果の概要（和文）：私の研究は、鋼鉄や他の金属の機械的特性、例えば強度や耐久性の向上に貢献しています。鋼の改良は、幅広い分野の研究であり、新しいタイプの鋼を開発する科学者たちは、理論的なガイドラインに頼っています。しかし、鋼の場合、これらのガイドラインを開発することは難しいです。鋼の屈曲は多くの相互作用する微視的プロセスの結果であり、これらのプロセスの集団行動の計算可能な記述を導き出す必要があります。私の研究は、これまでの記述を進化させ、より制限の少ないシナリオに適用できるようにしました。

研究成果の学術的意義や社会的意義
鉄や他の金属は建築物、インフラ、車両などの構築に使用されています。したがって、さらに小さな改良をすることが地球の資源保護、交通安全、および交通による汚染に膨大な影響を与えます。私の研究は、そのような改善の理論的な端に貢献しています。
また、私の研究の対応する数学的結果は、完全に異なる他の応用にも役立ちます。例えば、超伝導体（渦の群）、粒状媒体、動物の群れの移動、さらには人の集団の移動です。

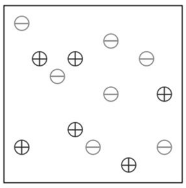
研究成果の概要（英文）：My research has contributed to the improvement of steel and other metals in terms of their mechanical properties such as strength and durability. Improving steel is a huge interdisciplinary field of research. Scientists who develop new types of steel rely on theoretical guidelines to improve steel. These guidelines are usually developed by engineers. However, in the case of steel these guidelines are difficult to develop. The main reason is that the bending of steel is the result of many interacting microscopic processes happening inside steel. It is therefore necessary to derive a computable description for the group behavior of these processes. My research has advanced previous descriptions such that they are applicable to less restrictive scenarios.

研究分野：関数方程式

キーワード：multiscale problems　plasticity　dislocations　particle systems

１．研究開始当初の背景

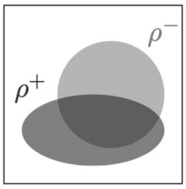
The background and motivation are written on the previous page. However, to describe the purpose, research methods and achievements, it is necessary to describe the background and setting in a mathematical manner.
In the description of the background I mention that my research is about deriving the group behavior of interacting microscopic processes inside steel. These microscopic processes are so-called *dislocations* which move through the steel. The easiest way to understand what dislocations are is to Google ‘dislocations in metal’. Here I give a brief description. Metals are formed by atoms that are stacked in an easy, regular pattern, like oranges in a box. However, in the case of metals, this stacking contains irregularities at various positions. An important type of such irregularities are called dislocations.
For the purpose of my research, we need to describe the movement of these dislocations through the steel. The actual movement is very difficult to describe. In order to make progress and to derive the group behavior, we need to use simplified descriptions for this movement.
One of the simplified descriptions that I use in my research is illustrated in the diagram below. The top left figure illustrates the dislocations in a squared domain (d = 2) as circles with a plus or a minus in it. The plus or minus denotes the orientation (or *sign*) of the dislocation.



$$(P_n): \quad \frac{dx_i}{dt} = -\frac{1}{n}\sum_{\substack{j=1 \\ j\neq i}}^{n} q_i q_j \nabla V(x_i - x_j) \quad t>0,\ i=1,\ldots,n$$

$\downarrow n \to \infty$

n	number of dislocations	x_i	position in $\mathbb{R}^d$ of dislocation i
d	dimension (≥ 1)	q_i	**sign** ($+1$ or -1) of dislocation i
$*$	convolution	$\rho^{\pm}$	pos./neg. particle density
V	**nonlocal, singular** interaction potential; $V(x) \to \infty$ as $x \to 0$		



$$(P): \quad \begin{cases} \partial_t \rho^+ = \operatorname{div}\big(\rho^+[\nabla V * (\rho^+ - \rho^-)]\big) & \text{on } \mathbb{R}^d,\ t>0 \\ \partial_t \rho^- = \operatorname{div}\big(\rho^-[\nabla V * (\rho^- - \rho^+)]\big) & \text{on } \mathbb{R}^d,\ t>0 \end{cases}$$

When time elapses, all dislocations will move around. This movement is described by the formula in the top of the diagram, which is called (P_n). In this description we assign a number to each dislocation such that we can distinguish them. I use the symbol i to denote this number. On the left of the equation is the velocity of dislocation i. The expression on the right describes this velocity in terms of the positions of all the other dislocations. It simply says that the velocity is given by the sum of the forces that each other dislocation exerts on dislocation i. This interaction force is such that dislocations of the same sign repel each other while dislocations of opposite sign attract each other with the same force. Since (P_n) has to hold for each dislocation i, it describes the movement of all dislocations.
Unfortunately, we cannot solve (P_n) exactly. We can solve it with a computer, but the computation time becomes very large when the number of dislocations is large (as is the case for steel). Therefore, the goal of my research is to approximate (P_n) by a different system, which is easier to understand and for which we can compute the solution in a reasonable amount of time. This system is (P), given in the lower part of the diagram. It describes how the *density* of the positive dislocations and the *density* of the negative dislocations move in time. The details of this description do not matter for the current explanation. The two densities depend both on time and space. Given a time point and a point in space, their value says how many dislocations there are per unit area around the given point in space. Therefore, (P) describes the *group behavior* of the dislocations; it cannot distinguish individual dislocations anymore, but it does describe in detail how the number of dislocations per unit area varies in time and space.

２．研究の目的

The purpose of the research is to *derive rigorously* the system (P) from (P_n). Such a derivation guarantees that there is precisely one system (P) which approximates (P_n) better and better as n increases. This statement can be formulated as a mathematical *limit* theorem, and the derivation of it is the proof of this theorem.
Recall that (P_n) is just one possible simplified description of dislocation dynamics. In fact, there are many different versions of (P_n) possible. Different descriptions are obtained by considering a different spatial dimension, considering dynamics versus the equilibrium states, considering dislocations with the same orientation, considering external forces acting on the dislocations, considering the influence of the boundary of the domain on the dislocation, including the effect of temperature, etc.
Once (P) is obtained as the limit of a certain (P_n), the next task is to try to build further on the corresponding derivation by extending it to more complex but less simplified version of (P_n). This is how my research has progressed in this project, where each step has resulted in one or more papers; see Section 5 below.
At the start of my project, a lot of limits from versions of (P_n) to (P) had already been obtained by other mathematicians and myself. Based on that, my research proposal focused on the following three specific subjects:

(1) Adding collisions to (P_n). Dislocations of opposite sign collide with each other. Upon collision, they cancel each other out and vanish. With these collisions there was no limit theorem yet.
(2) Adding the effect of the atoms and temperature to (P_n). In this description the dislocations are not free to move in any direction, but rather hop from one empty space in between atoms to a neighboring empty space. The temperature variable dictates how easy and how often these jumps occur. Also for this version of (P_n) there was no limit theorem yet.
(3) Quantifying the approximation. The usual type of limit theorem does not *quantify* how many particles are necessary for (P) to be a good approximation for (P_n). Yet, the number of dislocations in steel is finite (a typical order of magnitude is 10^5), and thus we want a more precise statement which tells us that for 10^5 dislocations (P) is a good approximation for (P_n). Such statement was not available yet for any version of (P_n).

３．研究の方法

The main research method was to sit in my office and try to connect together a large and complicated network of mathematical arguments which ultimately forms the proofs of the limit theorems of my research. This requires access to books and papers on related topics. To speed up this process and to prevent me from getting stuck I have worked together with mathematicians inside and outside of Japan. Thanks to these collaborations I have discovered much more than I would have been able to do alone. To facilitate these collaborations I have made research visits to my collaborators and have invited them to my home institute which is Kanazawa University.
I have also participated in various conferences, workshops and seminars in mathematical departments of universities. Such events foster the exchange of the latest research and trends in mathematics. It is vital for getting feedback on my own research, but also for obtaining new ideas on the key mathematical arguments required in my research.
Another method for figuring out whether a supposed limit theorem is true or false is to solve (P_n) and (P) on a computer. Doing this requires the development of new numerical codes. I have recruited Master students for developing, testing and refining these codes, which have turned into suitable Master projects for them.

４．研究成果

I split my achievements in four topics; the three specific subjects mentioned in Section 2 above (same numbering), and a fourth topic on unexpected results that came along the way:

(1) I solved this problem with my two collaborators Prof. Peletier and Dr. Pozar in one spatial dimension. This was a major result, because collisions happen at infinite speed, which falls beyond the scope of the usual mathematical theory. We obtained it by developing innovative arguments relying on some hidden features of (P_n) and (P). I think that this is a valuable addition to the mathematical field on particle systems, not only for building further on more complex versions of (P_n), but also for particle systems with applications other than steel.
Based on this paper I achieved two further results; one paper with Ms.c. Apisornpanich on a numerical method for solving (P), and one paper with Dr. Patrizi to connect (P_n) to a phase-field version of (P_n), again in terms of a limit theorem.
The future prospect is to complete a third paper which extends the limit theorem to a large class of different particle interaction forces, such that the results also apply to dislocation structures and other kinds of particle systems.
Another future goal is to extend to two spatial dimensions. This is very challenging, because the results above strongly rely on the one dimensional setting, and thus new techniques have to be developed.

(2) With collaborators Dr. Hudson and Prof. Peletier I have published a paper in which we establish a limit theorem in this setting. Actually, this limit theorem is quantitative in the sense described in (3) above. This is a major result that sets the stage for several possible follow-up studies in which (P_n) can be enriched.
There are two caveats though. First, we had to alter the interaction force so that it does not cause infinite collision speeds. Second, we think that our quantitative estimates are far from optimal.
Yet, I prefer to think of these caveats as future opportunities. Both can easily be explored computationally, simply by solving (P_n) and (P) numerically. However, this requires a careful setup and the development of new and efficient codes, which is a long project in the making which comprises of many Master projects put together.
In addition, without altering the interaction force there are recent advances in mathematics (on chemotaxis models) which seem to give new arguments by which a limit theorem can be proved. I am pursuing this direction at the very moment.

(3) With collaborator Prof. Kimura I found the first quantification for the approximation of (P_n) by (P). Since this is the first result, we did this in the easiest setting of (P_n): single sign, one dimension, and in equilibrium. While I have not found a way yet to extend this result to more complex versions of (P_n), I have obtained two new results based on the paper. The first is a single author paper in which I solve a previously open problem in one of my previous papers on boundary layers. The second is an improvement on estimates in function approximation theory, which is reported in a paper with Dr. Tanaka, who is an expert in this field.

(4) I published 6 other papers, which are all achievements related to the current research project. Next I describe these in more detail.
For subject (1) a deep understanding of singular ODEs is required. While studying this I got myself involved in two other projects in this field; one resulted in a paper with Dr. de Jong and one resulted in a paper with Prof. Kimura and Ms.c. Yang.
When studying subject (2), I came in touch with the Japanese group working on hydrodynamic limits of stochastic particle systems. I got interested, started to collaborate with Prof. Funaki, Prof. Sethuraman and Dr. Tsunoda, and wrote 2 papers with all three mathematicians.
The final two papers were sparked by discussions with other mathematicians working on dislocations and *disclinations* (another kind of irregularity in the stacking order of metallic atoms). The first is a single author paper on a simple but effective manner in which the self-interaction force of a dislocation *loop* can be described. The second is in collaboration with Dr. Cesana on the derivation of a mathematical framework in which disclinations can be described.

５．主な発表論文等

〔雑誌論文〕　計14件（うち査読付論文　14件／うち国際共著　13件／うちオープンアクセス　1件）

１．著者名 de Jong Thomas Geert、van Meurs Patrick	４．巻 180
２．論文標題 Uniqueness of Local, Analytic Solutions to Singular ODEs	５．発行年 2022年
３．雑誌名 Acta Applicandae Mathematicae	６．最初と最後の頁 1～13
掲載論文のDOI（デジタルオブジェクト識別子） 10.1007/s10440-022-00517-7	査読の有無 有
オープンアクセス オープンアクセスではない、又はオープンアクセスが困難	国際共著 該当する

１．著者名 van Meurs Patrick、Peletier Mark A.、Pozar Norbert	４．巻 246
２．論文標題 Discrete-to-Continuum Convergence of Charged Particles in 1D with Annihilation	５．発行年 2022年
３．雑誌名 Archive for Rational Mechanics and Analysis	６．最初と最後の頁 241～297
掲載論文のDOI（デジタルオブジェクト識別子） 10.1007/s00205-022-01812-1	査読の有無 有
オープンアクセス オープンアクセスとしている（また、その予定である）	国際共著 該当する

１．著者名 van Meurs Patrick、Tanaka Ken'ichiro	４．巻 29
２．論文標題 Convergence rates for energies of interacting particles whose distribution spreads out as their number increases	５．発行年 2023年
３．雑誌名 ESAIM: Control, Optimisation and Calculus of Variations	６．最初と最後の頁 1～28
掲載論文のDOI（デジタルオブジェクト識別子） 10.1051/cocv/2022083	査読の有無 有
オープンアクセス オープンアクセスではない、又はオープンアクセスが困難	国際共著 該当する

１．著者名 Kimura M.、van Meurs P.、Yang Z. X.	４．巻 174
２．論文標題 Particle Dynamics with Elastic Collision at the Boundary: Existence and Partial Uniqueness of Solutions	５．発行年 2021年
３．雑誌名 Acta Applicandae Mathematicae	６．最初と最後の頁 1~26
掲載論文のDOI（デジタルオブジェクト識別子） 10.1007/s10440-021-00423-4	査読の有無 有
オープンアクセス オープンアクセスではない、又はオープンアクセスが困難	国際共著 該当する

1．著者名	4．巻
Cesana Pierluigi、van Meurs Patrick	27
2．論文標題	5．発行年
Discrete-to-continuum limits of planar disclinations	2021年
3．雑誌名	6．最初と最後の頁
ESAIM: Control, Optimisation and Calculus of Variations	23～23
掲載論文のDOI（デジタルオブジェクト識別子）	査読の有無
10.1051/cocv/2021025	有
オープンアクセス	国際共著
オープンアクセスではない、又はオープンアクセスが困難	該当する

1．著者名	4．巻
van Meurs Patrick	26
2．論文標題	5．発行年
The continuum limit of interacting dislocations on multiple slip systems	2020年
3．雑誌名	6．最初と最後の頁
ESAIM: Control, Optimisation and Calculus of Variations	102～102
掲載論文のDOI（デジタルオブジェクト識別子）	査読の有無
10.1051/cocv/2020038	有
オープンアクセス	国際共著
オープンアクセスではない、又はオープンアクセスが困難	該当する

1．著者名	4．巻
Hudson Thomas、van Meurs Patrick、Peletier Mark	30
2．論文標題	5．発行年
Atomistic origins of continuum dislocation dynamics	2020年
3．雑誌名	6．最初と最後の頁
Mathematical Models and Methods in Applied Sciences	2557～2618
掲載論文のDOI（デジタルオブジェクト識別子）	査読の有無
10.1142/S0218202520500505	有
オープンアクセス	国際共著
オープンアクセスではない、又はオープンアクセスが困難	該当する

1．著者名	4．巻
Kimura Masato、van Meurs Patrick	53
2．論文標題	5．発行年
Quantitative Estimate of the Continuum Approximations of Interacting Particle Systems in One Dimension	2021年
3．雑誌名	6．最初と最後の頁
SIAM Journal on Mathematical Analysis	681～709
掲載論文のDOI（デジタルオブジェクト識別子）	査読の有無
10.1137/20M1322054	有
オープンアクセス	国際共著
オープンアクセスではない、又はオープンアクセスが困難	該当する

１．著者名 van Meurs Patrick	４．巻 33
２．論文標題 Expansions for the linear-elastic contribution to the self-interaction force of dislocation curves	５．発行年 2021年
３．雑誌名 European Journal of Applied Mathematics	６．最初と最後の頁 1032～1061
掲載論文のDOI（デジタルオブジェクト識別子） 10.1017/S0956792521000322	査読の有無 有
オープンアクセス オープンアクセスではない、又はオープンアクセスが困難	国際共著 該当する

１．著者名 van Meurs Patrick	４．巻 54
２．論文標題 Boundary-Layer Analysis of Repelling Particles Pushed to an Impenetrable Barrier	５．発行年 2022年
３．雑誌名 SIAM Journal on Mathematical Analysis	６．最初と最後の頁 1742～1774
掲載論文のDOI（デジタルオブジェクト識別子） 10.1137/21M1420198	査読の有無 有
オープンアクセス オープンアクセスではない、又はオープンアクセスが困難	国際共著 該当する

１．著者名 Funaki Tadahisa、van Meurs Patrick、Sethuraman Sunder、Tsunoda Kenkichi	４．巻 190
２．論文標題 Motion by Mean Curvature from Glauber-Kawasaki Dynamics with Speed Change	５．発行年 2023年
３．雑誌名 Journal of Statistical Physics	６．最初と最後の頁 1~30
掲載論文のDOI（デジタルオブジェクト識別子） 10.1007/s10955-022-03044-9	査読の有無 有
オープンアクセス オープンアクセスではない、又はオープンアクセスが困難	国際共著 該当する

１．著者名 Funaki Tadahisa、van Meurs Patrick、Sethuraman Sunder、Tsunoda Kenkichi	４．巻 38
２．論文標題 Constant-speed interface flow from unbalanced Glauber-Kawasaki dynamics	５．発行年 2023年
３．雑誌名 Ensaios Matematicos	６．最初と最後の頁 223~248
掲載論文のDOI（デジタルオブジェクト識別子） 10.21711/217504322023/em388	査読の有無 有
オープンアクセス オープンアクセスではない、又はオープンアクセスが困難	国際共著 該当する

１．著者名 van Meurs Patrick、Patrizi Stefania	４．巻 56
２．論文標題 Discrete Dislocation Dynamics with Annihilation as the Limit of the Peierls-Nabarro Model in One Dimension	５．発行年 2024年
３．雑誌名 SIAM Journal on Mathematical Analysis	６．最初と最後の頁 197～233
掲載論文のDOI（デジタルオブジェクト識別子） 10.1137/22M1527052	査読の有無 有
オープンアクセス オープンアクセスではない、又はオープンアクセスが困難	国際共著 該当する

１．著者名 Apisornpanich Lalita, van Meurs Patrick	４．巻 66
２．論文標題 A simple, accurate scheme for the flow of an electric charge distribution	５．発行年 2023年
３．雑誌名 The Science Reports of Kanazawa University	６．最初と最後の頁 1~16
掲載論文のDOI（デジタルオブジェクト識別子） 10.24517/0002000263	査読の有無 有
オープンアクセス オープンアクセスではない、又はオープンアクセスが困難	国際共著 －

〔学会発表〕　計13件（うち招待講演　10件／うち国際学会　6件）

１．発表者名 van Meurs, Patrick
２．発表標題 Atomistic origins of continuum dislocation dynamics
３．学会等名 15th World Congress on Computational Mechanics（招待講演）（国際学会）
４．発表年 2022年

１．発表者名 van Meurs, Patrick
２．発表標題 Huygens' principle from unbalanced Glauber-Kawasaki dynamics
３．学会等名 SALSIS workshop on stochastic analysis（招待講演）
４．発表年 2022年

1．発表者名 van Meurs, Patrick
2．発表標題 Scaling limits of a nonlocally interacting particle system
3．学会等名 Workshop on Probabilistic Methods in Statistical Mechanics of Random Media and Random Fields 2023（招待講演）（国際学会）
4．発表年 2023年

1．発表者名 van Meurs Patrick
2．発表標題 Discrete-to-continuum convergence of charged particles in 1D with annihilation
3．学会等名 Kyoto Applied Math seminar（招待講演）
4．発表年 2021年

1．発表者名 van Meurs Patrick
2．発表標題 Discrete-to-continuum limit of dislocation dynamics including collisions
3．学会等名 SIAM Conference on Mathematical Aspects of Materials Science（国際学会）
4．発表年 2021年

1．発表者名 van Meurs Patrick
2．発表標題 Convergence rates of interacting particle systems in the many particle limit
3．学会等名 SIAM Conference on Mathematical Aspects of Materials Science（国際学会）
4．発表年 2021年

１．発表者名
van Meurs Patrick

２．発表標題
Hydrodynamic limit for Glauber-Kawasaki dynamics with speed change

３．学会等名
SALSIS workshop on stochastic analysis（招待講演）

４．発表年
2021年

１．発表者名
van Meurs Patrick

２．発表標題
Hydrodynamic limit for a stochastic interacting particle system on the discrete torus

３．学会等名
Kanazawa Analysis Seminar（招待講演）

４．発表年
2022年

１．発表者名
van Meurs Patrick

２．発表標題
Quantification of the difference between discrete and continuum descriptions of arrays of dislocations

３．学会等名
Cardiff School of Mathematics Seminar（招待講演）

４．発表年
2021年

１．発表者名
van Meurs Patrick

２．発表標題
Mean curvature flow as the limit of a spin system

３．学会等名
10th International Congress on Industrial and Applied Mathematics (ICIAM)（国際学会）

４．発表年
2023年

１．発表者名 van Meurs Patrick
２．発表標題 Plasticity as the collective motion of lattice defects
３．学会等名 Applied Mathematics Seminar at University of New South Wales（招待講演）（国際学会）
４．発表年 2023年

１．発表者名 van Meurs Patrick
２．発表標題 Towards a particle system for the incompressible Navier-Stokes equation
３．学会等名 SALSIS workshop on stochastic analysis（招待講演）
４．発表年 2023年

１．発表者名 van Meurs Patrick
２．発表標題 Convergence of a phases-field model to a system of moving particles (P) in 1D with collisions
３．学会等名 Workshop on nonlinear Analysis（招待講演）
４．発表年 2023年

〔図書〕　計0件

〔産業財産権〕

〔その他〕

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7．科研費を使用して開催した国際研究集会

〔国際研究集会〕　計0件

8．本研究に関連して実施した国際共同研究の実施状況

共同研究相手国	相手方研究機関