Peer Review Information

Journal: Nature Computational Science
Manuscript Title: Fast kinetic simulator for relativistic matter
Corresponding author name(s): Daniele Simeoni

Reviewer Comments & Decisions:

Decision Letter, initial version:

Message: ** Please ensure you delete the link to your author homepage in this e-mail if you wish to forward it to your co-authors. **

Dear Dr Simeoni,

Your manuscript "Fast kinetic simulator for relativistic matter" has now been seen by 3 referees, whose comments are appended below. You will see that while they find your work of interest, they have raised points that need to be addressed before we can make a decision on publication.

The referees' reports seem to be quite clear. Naturally, we will need you to address all of the points raised.

While we ask you to address all of the points raised, the following points need to be substantially worked on:
- As suggested by referees, please enrich your method discussions. You could use the Methods section where we do not have a strict word limit.
- Please clarify the novelty and technical details of your methods, as suggested by referees.
- Please stress your contributions when compared with previous work via experiments.
- Please include more evidence to demonstrate the computational efficiency.

- Please follow referee #3's suggestion to broaden the scope of your method and apply it to other important problems.

Please use the following link to submit your revised manuscript and a point-by-point response to the referees' comments (which should be in a separate document to any cover letter):

[REDACTED]

** This url links to your confidential homepage and associated information about manuscripts you may have submitted or be reviewing for us. If you wish to forward this e-mail to co-authors, please delete this link to your homepage first. **

To aid in the review process, we would appreciate it if you could also provide a copy of your manuscript files that indicates your revisions by making of use of Track Changes or similar mark-up tools. Please also ensure that all correspondence is marked with your Nature Computational Science reference number in the subject line.

In addition, please make sure to upload a Word Document or LaTeX version of your text, to assist us in the editorial stage.

If you have any issues when updating your Code Ocean capsule during the revision process, please email the Code Ocean support team Cc'ing me.

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We hope to receive your revised paper within three weeks. If you cannot send it within this time, please let us know.

We look forward to hearing from you soon.

Best regards,

Jie Pan, Ph.D.
Associate Editor
Nature Computational Science

Reviewers comments:

Reviewer #1 (Remarks to the Author):

This paper concerns kinetic simulators for relativistic flows, extending previous lattice simulation beyond the fluid regime towards dilute gases. Conceptually, this is a very important problem. It also poses severe technical challenges for a numerical scheme. The examples provided in the paper suggests that the model performs very well - perhaps better than one might have expected. The results are interesting and relevant, especially as

they point towards the ability to simulate problems that evolve from one regime to another. I can think of many topical problems where this kind of scheme could be put to use.

The paper is well written, with clear presentation and illustrative examples. Having read it, I was certainly convinced by the merits of the new scheme. The one thing I found slightly annoying was the forward reference to the method - finally presented in section V. I understand why this is done, but the authors would be well advised to add a few more sentences on the method in section IIA. Other than that, I think the logic was easy to follow.

In short, this is an interesting and relevant contribution to the literature. I am very happy to support its publication.

Reviewer #2 (Remarks to the Author):

The manuscript under review is discussing relativistic lattice Boltzmann simulations for strongly and weakly interacting systems.

The main innovation that the authors report is that they have improved the momentum integration of the rel. lattice Boltzmann technique by using a higher order scheme.

The authors demonstrate the quality of their implementation by comparing their simulations to calculations using the relativistic parton cascade model BAMPS developed nearly two decades ago by Greiner and Xu.

The main claims of the authors are:
- their lattice Boltzmann approach can treat fluids and gases,
- their approach can be used to simulate massive and massles gases,
- their approach is very fast.

While the method is indeed elegant and the manuscript seems free of any errors, I have further questions that would need to be clarified:
1.
The description of the method is rather short and should be extended.

2.
I can not really see the innovative character of the proposed method. There are various numerical methods to solve the equations of motion of viscous fluids, ranging from standard solvers like the SHASTA and other schemes like Kurganov-Tadmore, etc. to finite element methods to particle simulations. Especially particle based simulations define the prime standard here. BAMPS is an excellent example and is also used by the authors as a benchmark.

This reinforces my main problem: lack of innovation. BAMPS is 20 years old and can since then treat fluids and gases (actually even out of equilibrium in contrast to the lattice Boltzmann method which relies on the relaxation time approximation). BAMPS can also simulate massive and massless particles. BAMPS could be very fast when ran on parallel computers. So why not just run BAMPS?

I also do not see that the simulation times presented in the manuscript are especially short. Speed-ups of hydrodynamic codes, when put on graphic cards have easily been on the level of factors 100-1000 compared to CPU running times (see J. Gerhard, Comput.Phys.Commun. 184 (2013) 311-319). Also the absolute simulation times seem to

3

be comparable to the old results by Gerhard et al. So where is the improvement?

To summarize, I think all results presented in the manuscript are correct. However, I do not see anything special and innovative in the manuscript.
Therefore, I do not recommend publication of the current manuscript, but await further answers by the authors.

Reviewer #3 (Remarks to the Author):

The present manuscript describes a new and fast numerical method to solve the bulk dynamics of relativistic matter, for interaction parameters ranging from the fluid dynamic to (almost) ballistic regime.

Executive summary: In my opinion, this work constitutes a major step forward in simulating the dynamics of relativistic matter. Specifically the ability to solve the dynamics over a wide range of Knudsen numbers is superior to any other solvers currently on the market. This differs markedly from the state-of-the-art of solvers that are limited to only the fluid or only the ballistic regime. As a consequence, I expect the approach described in the present paper to lead to break-through discoveries in the difficult-to-simulate regime of intermediate Knudsen number flows. For this reason, I strongly suggest publication of the manuscript in Nature Computational Science after minor revisions.

Detailed report:

Concerning validity of the method, the authors presented comparison of their numerical approach to analytic test cases, such as the Riemann problem, finding excellent agreement. Furthermore, they presented comparison between their numerical approach and a particle-based approach in Fig.4, finding again excellent agreement. Since these are very non-trivial tests of the author's numerical approach, the method, and as a consequence the results, are likely to be valid.

The authors conclude by saying that their method allows for 'computationally efficient large-scale simulations of beyond-hydrodynamic regimes in the framework of QGP experiments'. I agree with this conclusion, but find their focus to be too narrow. While application of their method to QGP experiments is one potential goal, there are other systems where a computational tool such as the one presented in the present study is even more pressing. For instance, in plasma physics the question of entropy production in a (almost) collisionless plasma is unresolved, see e.g. Zhdankin's work

https://arxiv.org/pdf/2110.07025.pdf

Other potential applications of this approach could be proto-neutron stars where the neutrinos are initially trapped inside, but almost free-stream through the outer layers of the star. So while I support the author's conclusion, I think they should broaden their scope in the conclusion and point out other physics systems where their tool is not only nice, but CRUCIAL to solving the problem.

Suggested improvements:

1) page 3: the BRAHMS experiment is misspelled; also, all of the QGP experiments listed no longer exist. The authors should include the relevant LHC experiments

2) page 10: Bjorken attractor [34]. While [34] is indeed dealing with the Bjorken attractor, I would have expected some other references as well. In particular, I would have expected the authors to cite Heller and Spalinski for the 'hydro' attractor

https://arxiv.org/pdf/1503.07514.pdf

Furthermore, the authors may find the analytic approximation (4) for the RTA attractor useful:

https://arxiv.org/pdf/1704.08699.pdf

Finally, there is a recent review on attractors by Soloviev:

https://arxiv.org/pdf/2109.15081.pdf

3) page 10: missing reference after "particle yields"

4) Discussion: in addition to broadening the focus of applications of the new tool, I would like to point out a key problem in current simulations of QGP systems, namely hadronization. Specifically, while fluid dynamic simulations of the 'hot' fireball work well, and while parton-cascade simulations of the 'cold' hadrons work well, one would like to have a single simulation of BOTH phases at the same time. This is currently not feasible because up to date, no single algorithm can handle both the fluid and gas phase simultaneously, but it seems to be as if the present approach could be the right tool for the job. As a simple test and follow-up work, the authors could consider simulating so-called cavitation, which is believed to signal the onset of hadronization in QCD. For some random references on the subject, have a look at

https://arxiv.org/pdf/0908.1785.pdf
https://arxiv.org/pdf/1405.1978.pdf
https://arxiv.org/pdf/1910.12930.pdf

5) Discussion: another poorly understood feature in heavy-ion collisions is the large pT behavior of collective flow. Usually this is again attributed to the transition from fluid dynamics to the ballistic regime, but there is a clear trend in the experimental data, see e.g. Fig 8 rhs in

https://arxiv.org/pdf/1801.03477.pdf

As another follow-up project, the authors could consider simulating collective flow for ALL pT. While a full QGP simulation may be too daunting to implement, a strong step in this direction would be to fill in the dashed lines for Fig.4 lhs in

https://arxiv.org/pdf/1802.06804.pdf

and potentially elucidate the connection between the peak in v_n(pT) and the location of the first non-hydrodynamic mode

6) Methods, subsection C. For massless particles, it seems to me that the discretization scheme is similar to

https://arxiv.org/pdf/1106.1093.pdf
https://arxiv.org/pdf/2101.06187.pdf

Can the authors discuss what the differences are between their discretization scheme and those (if any)?

Signed report: Paul Romatschke

Author Rebuttal to Initial comments

Dear Editor,

please find attached a revised version of the manuscript "Fast kinetic simulator for relativistic matter".

This new version has been changed in order to account for the comments made by the referees. As explained below, we have carefully addressed all questions raised by the referees and we hope that this improved version can now be published in "Nature Computational Science".

In what follows we address in details all issues raised by Referees #1, #2 and #3, with our replies also including a description of the corresponding changes made in the paper.

I.   REPORT OF REFEREE 1

This paper concerns kinetic simulators for relativistic flows, extending previous lattice simulation beyond the fluid regime towards dilute gases. Conceptually, this is a very important problem. It also poses severe technical challenges for a numerical scheme. The examples provided in the paper suggests that the model performs very well - perhaps better than one might have expected. The results are interesting and relevant, especially as they point towards the ability to simulate problems that evolve from one regime to another. I can think of many topical problems where this kind of scheme could be put to use.

The paper is well written, with clear presentation and illustrative examples. Having read it, I was certainly convinced by the merits of the new scheme. The one thing I found slightly annoying was the forward reference to the method - finally presented in section V. I understand why this is done, but the authors would be well advised to add a few more sentences on the method in section IIA. Other than that, I think the logic was easy to follow.

Reply: The format of the journal requires that Methods be introduced at the end of the article, therefore we have placed a more detailed explanation in that section.

Nevertheless, we have taken into account the referee recommendation by adding a few comments on the method in Sec. IIA, where we introduce and clarify the meaning of the parameters that are used throughout the remaining part of the article.

Furthermore, additional details have been provided also in the Methods section.

In short, this is an interesting and relevant contribution to the literature. I am very happy to support its publication.

Reply: We wish to thank the referee for her/his valuable and appreciative remarks.

II. REPORT OF REFEREE 2

The manuscript under review is discussing relativistic lattice Boltzmann simulations for strongly and weakly interacting systems.

The main innovation that the authors report is that they have improved the momentum integration of the rel. lattice Boltzmann technique by using a higher order scheme.

The authors demonstrate the quality of their implementation by comparing their simulations to calculations using the relativistic parton cascade model BAMPS developed nearly two decades ago by Greiner and Xu.

The main claims of the authors are:

- *their lattice Boltzmann approach can treat fluids and gases,*

- *their approach can be used to simulate massive and massles gases,*

- *their approach is very fast.*

While the method is indeed elegant and the manuscript seems free of any errors, I have further questions that would need to be clarified:

1. The description of the method is rather short and should be extended.

Reply: Further details on the numerical method have been added to the Methods section at the end of the paper.

2. I can not really see the innovative character of the proposed method. There are various numerical methods to solve the equations of motion of viscous fluids, ranging from standard solvers like the SHASTA and other schemes like Kurganov-Tadmore, etc. to finite element methods to particle simulations. Especially particle based simulations define the prime standard here. BAMPS is an excellent example and is also used by the authors as a benchmark.

Reply: Following the referee recommendation, additional references have been inserted in the main text, for both relativistic hydro-codes and particle-based solvers.

This reinforces my main problem: lack of innovation. BAMPS is 20 years old and can since then treat fluids and gases (actually even out of equilibrium in contrast to the lattice Boltzmann method which relies on the relaxation time approximation). BAMPS can also simulate massive and massless particles. BAMPS could be very fast when ran on parallel computers. So why not just run BAMPS?

Reply: We thank the referee for providing us with the opportunity to clarify a number of important points.

First and foremost, we wish to emphasize that RLB is no replacement for BAMPS; it is however a very convenient alternative whenever BAMPS proves to be a computational overkill, i.e. for mildly non-equilibrium situations which escape a hydro description but do not yet require a full kinetic treatment. Within this context, RLB is generally about two orders of magnitude faster than BAMPS as personally experienced by one of the authors (VEA) for the case of 0+1D and 2+1D Bjorken flow simulations (see Ref. [45] in the revised manuscript). In single-core runtime hours, for the former case, RLBM takes about 30 seconds to run, while BAMPS takes around 30 minutes to gather sufficient statistics. In the latter case, RLBM takes less than 2h, while BAMPS takes around 30h for one run. This is only natural, since BAMPS contains much more non-equilibrium physics, which means that the above figures should not be regarded as competitive remarks, but as a statement of complementarity instead.

We also wish to call the referee's attention on the fact that classical (non-relativistic) LB has played a very analogue role versus molecular dynamics (MD), see for instance:

J. Horbach, S. Succi, *Lattice Boltzmann versus molecular dynamics simulation of nanoscale hydrodynamic flows*, Phys. Rev. Lett. 96, 224503 (2006),

where it was shown that LB can capture nano-vorticity patterns at a tiny fraction of the cost of molecular dynamics simulations. Once again, obviously

LB cannot replace MD in general, but for problems where MD details are not needed, it cuts the MD costs by orders of magnitude. Spotting such opportunities is probably the most far-reaching contribution of LB to the physics of classical fluids, and this paper is meant to highlight a similar opportunity for the case of relativistic matter.

Summarizing, RLB is by no means a general replacement for BAMPS; yet it can serve eminently well for problems which do not demand full kinetic treatment, such as the ones discussed in this paper. This is why we sincerely believe that our paper makes a very sensible contribution, to the existing literature, as after all explicitly acknowledged by Reviewers 1 and 3.

To make the point crystal clear, we have inserted a clarifying comment at page 17 (section III _Performance data_) of the revised manuscript:

" Indeed, with suitable coupling to Monte Carlo schemes, by sampling particle position and momenta from the RLBM solution, [88], it may also be possible to describe the re-hadronization stage, in which quarks bind back into hadrons [20,22,89-91]. Compared to Monte-Carlo-based implementations such as BAMPS [19,23,45,92], which suffer from statistical noise, our scheme can be expected to be between 1 and 2 orders of magnitude faster."

I also do not see that the simulation times presented in the manuscript are especially short. Speed-ups of hydrodynamic codes, when put on graphic cards have easily been on the level of factors 100-1000 compared to CPU running times (see J. Gerhard, Comput.Phys.Commun. 184 (2013) 311-319). Also the absolute simulation times seem to be comparable to the old results by Gerhard et al. So where is the improvement?

Reply: We thank the reviewer for pointing out this reference, which we have now included as Ref. [14] in the revised manuscript. Fig. 5 therein indicates that SHASTA requires 30 s for 100 time steps in single precision on a 200^3 grid, or equivalently 26.67 MLUPS. This performance is achieved on the AMD 5870 GPU card, which does 2.72 TFLOPS according to its spec sheet. We employed the NVIDIA V100 card, which does 7 TFLOPS in double precision (this is what we used for the benchmark) and is thus $\simeq 2.57$ times faster. Scaling the results in Ref. [14] by this factor, the SHASTA would reach 68 MLUPS on the V100, about 15% faster than our $K = 7$ model employing 128 populations. Note that $K = 7$ is sufficient for simulations in the hydro regime, when $Kn \lesssim 0.1$, while the SHASTA solver in Eq. Ref. [14] solves the Euler equations involving 5 degrees of freedom

(n, ϵ and u^μ with normalization $u^2 = 1$). Taking into account that state-of-the-art hydro simulations involving viscous effects must solve the second-order evolution equations for 9 additional degrees of freedom (Π, V^μ and $\pi^{\mu\nu}$), it is not unreasonable to assume that the runtime of a (hypothetical) vSHASTA GPU implementation is larger by a factor of $\gtrsim 3$ compared to the SHASTA solver for the Euler equations. For example, in Ref. [53] we found that vHLLE is ~ 4 times slower when including viscous effects compared to the ideal fluid case, tested for the 2+1D Bjorken flow with transverse dynamics of an ultrarelativistic conformal fluid without conserved charges.

While we cannot substantiate the above discussion with concrete numbers, we hope that the referee will agree that our scheme is indeed competitive from a runtime perspective and can serve as an efficient alternative to standard hydro solvers, within its range of applicability. We added a comment in this respect in the first paragraph of Section III, which can be found on page 16 of the revised manuscript.

To summarize, I think all results presented in the manuscript are correct. However, I do not see anything special and innovative in the manuscript. Therefore, I do not recommend publication of the current manuscript, but await further answers by the authors.

Reply: We feel and hope that our clarifications fully address the referee's concerns. Again, thanks for inviting us, through stimulating remarks, to clarify the important matters above.

III. REPORT OF REFEREE 3

The present manuscript describes a new and fast numerical method to solve the bulk dynamics of relativistic matter, for interaction parameters ranging from the fluid dynamic to (almost) ballistic regime.

Executive summary: In my opinion, this work constitutes a major step forward in simulating the dynamics of relativistic matter. Specifically the ability to solve the dynamics over a wide range of Knudsen numbers is superior to any other solvers currently on the market. This differs markedly from the state-of-the-art of solvers that are limited to only the fluid or only the ballistic regime. As a consequence, I expect the approach described in the present paper to lead to break-through discoveries in the difficult-to-simulate regime of intermediate Knudsen number flows. For this reason, I strongly suggest publication of the manuscript in Nature Computational Science after minor revisions.

Detailed report:

Concerning validity of the method, the authors presented comparison of their numerical approach to analytic test cases, such as the Riemann problem, finding excellent agreement. Furthermore, they presented comparison between their numerical approach and a particle-based approach in Fig.4, finding again excellent agreement. Since these are very non-trivial tests of the author's numerical approach, the method, and as a consequence the results, are likely to be valid.

The authors conclude by saying that their method allows for 'computationally efficient large-scale simulations of beyond-hydrodynamic regimes in the framework of QGP experiments'. I agree with this conclusion, but find their focus to be too narrow. While application of their method to QGP experiments is one potential goal, there are other systems where a computational tool such as the one presented in the present study is even more pressing. For instance, in plasma physics the question of entropy production in a (almost) collisionless plasma is unresolved, see e.g. Zhdankin's work https://arxiv.org/pdf/2110.

Reply: We wish to thank the referee for her/his encouraging remarks and

highly valued suggestions. References to applications of the present method to near-collisionless plasmas have been added to the text.

Other potential applications of this approach could be proto-neutron stars where the neutrinos are initially trapped inside, but almost free-stream through the outer layers of the star. So while I support the author's conclusion, I think they should broaden their scope in the conclusion and point out other physics systems where their tool is not only nice, but CRUCIAL to solving the problem.

Suggested improvements:

1) page 3: the BRAHMS experiment is misspelled; also, all of the QGP experiments listed no longer exist. The authors should include the relevant LHC experiments

Reply: References to the correct LHC experiments have been added. Furthermore, the misspelling of the BRAHMS experiment has been fixed.

page 10: Bjorken attractor [34]. While [34] is indeed dealing with the Bjorken attractor, I would have expected some other references as well. In particular, I would have expected the authors to cite Heller and Spalinski for the 'hydro' attractor https://arxiv.org/pdf/1503.

Reply: Reference to Heller-Spalinski was already present in the text, but it has been moved to a more visible position.

Furthermore, the authors may find the analytic approximation (4) for the RTA attractor useful: https://arxiv.org/pdf/1704.

Reply: Thank you for this very useful suggestion. The analytic approximation for the Bjorken attractor found in https://arxiv.org/pdf/1704 has been added to fig.4, where it is shown that it overlaps with our numerical results.

Finally, there is a recent review on attractors by Soloviev: https://arxiv.org/pdf/2109.

Reply: reference added to the text. Thanks again.

2) page 10: missing reference after "particle yields"

Reply: the reference is now clearly evidenced.

3) Discussion: in addition to broadening the focus of applications of the new tool, I would

like to point out a key problem in current simulations of QGP systems, namely hadronization. Specifically, while fluid dynamic simulations of the 'hot' fireball work well, and while parton-cascade simulations of the 'cold' hadrons work well, one would like to have a single simulation of BOTH phases at the same time. This is currently not feasible because up to date, no single algorithm can handle both the fluid and gas phase simultaneously, but it seems to be as if the present approach could be the right tool for the job. As a simple test and follow-up work, the authors could consider simulating so-called cavitation, which is believed to signal the onset of hadronization in QCD. For some random references on the subject, have a look at

- https://arxiv.org/pdf/0908.1785.pdf

- https://arxiv.org/pdf/1405.1978.pdf

- https://arxiv.org/pdf/1910.12930.pdf

4) Discussion: another poorly understood feature in heavy-ion collisions is the large pT behavior of collective flow. Usually this is again attributed to the transition from fluid dynamics to the ballistic regime, but there is a clear trend in the experimental data, see e.g. Fig 8 rhs in https://arxiv.org/pdf/1801.03477.pdf

As another follow-up project, the authors could consider simulating collective flow for ALL p_T. While a full QGP simulation may be too daunting to implement, a strong step in this direction would be to fill in the dashed lines for Fig.4 lhs in https://arxiv.org/pdf/1802.06804.pdf and potentially elucidate the connection between the peak in $v_n(p_T)$ and the location of the first non-hydrodynamic mode

Reply: Thanks for providing such an informative and detailed feedback! A new paragraph discussing all possible follow ups has been added to the Discus- sion section. Furthermore, most of the references proposed by the referee have been added to the text.

5) Methods, subsection C. For massless particles, it seems to me that the discretization scheme is similar to

https://arxiv.org/pdf/1106.1093.pdf

https://arxiv.org/pdf/2101.06187.pdf

Can the authors discuss what the differences are between their discretization scheme and those (if any)?

Reply: Our RLB method is based on an assumption of particle number con- servation, via quadrature preservation of the particle flow in addition to the energy momentum tensor. The quadratures are built in such a way as to pre- serve more moments of the distribution function (indeed even more than the hydrodynamic ones, when tackling high Kn flows).

Furthermore, the angular discretization is performed differently with respect to https://arxiv.org/pdf/1106.1093, as in our approach we consider angular quadratures that correctly integrate spherical harmonics on the sphere (while in the mentioned papers angular product rules are used).

Decision Letter, first revision:

Dear Dr. Simeoni,

Thank you for submitting your revised manuscript "Fast kinetic simulator for relativistic matter" (NATCOMPUTSCI-22-0365A). It has now been seen by the original referees and their comments are below. The reviewers find that the paper has improved in revision, and therefore we'll be happy in principle to publish it in Nature Computational Science, pending minor revisions to satisfy the referees' final requests and to comply with our editorial and formatting guidelines.

We are now performing detailed checks on your paper and will send you a checklist detailing our editorial and formatting requirements in about a week. Please do not upload the final materials and make any revisions until you receive this additional information from us.

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Thank you again for your interest in Nature Computational Science Please do not hesitate to contact me if you have any questions.

Sincerely,

Jie Pan, Ph.D.
Associate Editor
Nature Computational Science

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Reviewer #1 (Remarks to the Author):

The authors have addressed my concerns. No further comments necessary.

Reviewer #2 (Remarks to the Author):

I thank the authors for clarifying my main question, namely the lack of innovation. With the newly provided information and the additional discussion in the text, I can clearly see the huge benefits of the proposed method.

Therefore, I am happy to support publication of the revised manuscript.

Reviewer #3 (Remarks to the Author):

I thank the authors for their detailed reply to my criticisms and their updated manuscript. I really like the latest version of the manuscript, and I recommend publication of the manuscript in its present form in Nature Computational Science.

Final Decision Letter:

Date: 8th September 22 03:21:18
Last Sent: 8th September 22 03:21:18
Triggered By: Jie Pan
From: jie.pan@us.nature.com
To: dan.simeoni@gmail.com
CC: gbblsn@unife.it
Subject: Decision on Nature Computational Science manuscript NATCOMPUTSCI-22-0365B
Message: Dear Dr Simeoni,

We are pleased to inform you that your Article "Fast kinetic simulator for relativistic matter" has now been accepted for publication in Nature Computational Science.

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