Adaptive Initiation of AutoPas Tuning Phases for Efficient Particle Simulations

Bachelor's Thesis in Informatics

Niklas Ladurner

Technische Universität München
School of Computation, Information and Technology - Informatics
Chair of Scientific Computing in Computer Science

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Adaptives Auslösen von Tuning-Phasen für effiziente Partikelsimulation in AutoPas

Bachelor's Thesis in Informatics

Niklas Ladurner

Supervisor: Univ.-Prof. Dr. Hans-Joachim Bungartz
Chair of Scientific Computing in Computer Science

Advisor: Manish Mishra, M.Sc.
Chair of Scientific Computing in Computer Science

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I confirm that this bachelor's thesis is my own work and I have documented all sources and material used.

Munich, 15.09.2025 Niklas Ladurner

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Acknowledgements

Writing Guidance

In the *Acknowledgment* section, express your gratitude to those who helped and supported your work. Start by thanking your advisors, mentors, or supervisors who provided guidance and expertise. Mention any colleagues, classmates, or team members who contributed to discussions or offered assistance. You can also acknowledge specific organisations, institutions, or funding sources that supported your research or work. Lastly, include any personal acknowledgments for family or friends who offered encouragement and moral support during the project. Keep this section sincere, concise, and professional.

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Abstract

Particle simulations have become an indispensable tool in research and are used across a wide range of applications. Depending on the specific scenario, different simulation configurations may be more suitable. AutoPas is a particle simulation library that offers a simple black-box interface for researchers. To achieve this, AutoPas reevaluates the optimal configuration at fixed intervals. This thesis proposes a dynamic approach to determine ideal points for the initiation of new tuning phases.

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Zusammenfassung

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1 Introduction and Background

This chapter will ...

1.1 Motivation

1.2 Particle simulation

2 Background

This chapter will ...

2.1 AutoPas

2.2 Section 2

3 Implementation

To dynamically initiate new tuning phases, a strategy must be found such that they can be triggered at runtime on live simulation data. Depending on the scenario and available statistics provided by the simulation, different strategies of finding these trigger points may be optimal. In this chapter therefore, the strategies investigated are presented.

3.1 Considerations

3.1.1 Computational overhead

3.1.2 Available simulation statistics

3.2 Time-based Triggers

The simplest approach in detecting whether the current configuration might become suboptimal is to observe changes in iteration runtime. As a specific configuration becomes less suitable as the simulation state changes, one would expect the runtime to increase, as e.g. suboptimal containers lead to unfavorable access patterns. Therefore, the primary focus of this thesis lies on runtime-based strategies in finding trigger points.

3.2.1 Simple Trigger

3.2.2 Single-iteration averaging Trigger

3.2.3 Interval averaging Trigger

3.2.4 Linear Regression Trigger

This approach is conceptually similar to the interval averaging trigger, with one major difference: Instead of comparing the current interval of runtimes to a previous one, it tries to estimate the runtime in the next interval based on data of the current interval and compares it that way ...

The general idea is to fit a simple linear regression, adapted to our use case, on the last n runtime samples. Using the linear regression we obtain a slope estimator $\hat{\beta}_1$, by which we can predict the runtime in the next interval. In the following, t_k is the runtime at iteration k, i the current iteration and $\bar{t}$, $\bar{k}$ the average runtime and iteration respectively. Then the slope estimator $\hat{\beta}_1$ in the standard simple linear regression model is presented in (3.1).

$$\hat{\beta}_1 = \frac{\sum_{k=i-n-1}^{i}(k-\bar{k})(t_k-\bar{t})}{\sum_{k=i-n-1}^{i}(k-\bar{k})^2}, \quad \bar{t} = \frac{1}{n}\sum_{k=i-n-1}^{i} t_k, \quad \bar{k} = \frac{1}{n}\sum_{k=i-n-1}^{i} k \tag{3.1}$$

The value of the estimator $\hat{\beta}_0$, i.e. the intersection at $y = 0$, is not of interest. Similarly, as the samples are taken in constant steps of one iteration, the values of k can be shifted to the interval $[0, n]$. Considering these two points, the model can be transformed to (3.2), where A, B are constants that can be precomputed at initialization, as given in (3.3).

$$\hat{\beta}_1' = \frac{\sum_{k=0}^{n-1}\left(k - \frac{n(n-1)}{2n}\right)(t_{i-n-1+k} - \bar{t})}{\sum_{k=0}^{n-1}\left(k - \frac{n(n-1)}{2n}\right)^2} = \frac{1}{B}\sum_{k=0}^{n-1}(k-A)(t_{i-n-1+k} - \bar{t}) \tag{3.2}$$

$$A = \frac{n-1}{2}, \quad B = \sum_{k=0}^{n-1}(k-A)^2 \tag{3.3}$$

$\hat{\beta}_1'$ can thus be interpreted as "in each iteration, the runtime is projected to increase $\hat{\beta}_1'$ nanoseconds". This however, is not a sensible metric to compare to a user-set triggerFactor, as it heavily depends on the scenario and would require to know rough iteration runtime estimates beforehand. Therefore, we use a normalization function, such that a factor of 1.0 is roughly equal to "no runtime increase". The resulting value is also consistent to other triggers. The normalization implemented is presented in (3.4).

$$\hat{\beta}_{\text{norm}} = \frac{n \cdot \hat{\beta}_1'}{\bar{t}} \tag{3.4}$$

In particular, we have:

- $\hat{\beta}_{\text{norm}} = 1$ if there is no projected change in iteration runtime
- $\hat{\beta}_{\text{norm}} > 1$ if there is a projected increase in iteration runtime
- $\hat{\beta}_{\text{norm}} < 1$ if there is a projected decrease in iteration runtime
- $\hat{\beta}_{\text{norm}} = 2$ if there the runtime of the next interval is projected to be double the current interval's runtime.

3.3 Hybrid Triggers

As will be discussed later, time-based approaches are not suitable for all scenarios. In these scenarios, iteration runtimes alone might not be a good enough indicator for scenario change. As AutoPas provides additional live simulation statistics through its `liveinfo` interface, these can be used in combination with iteration runtimes to find better strategies in detecting scenario change.

4 Evaluation

This chapter will present the scenarios and criteria used to evaluate our implementation. Additionally, the results of these benchmarks are reported.

4.1 Benchmarking Scenarios

As to not limit our analysis to one specific simulation setting, we use a selection of benchmarking scenarios. These represent different structures as they may be used in real-world applications. The heating-sphere and exploding-liquid scenarios are identical to the ones given by Newcome et al., the configuration files have been adapted and parametrized for use in this thesis [New+25]. The other scenarios are are taken from the AutoPas `md-flexible` example.

4.1.1 Equilibrium

In the equilibrium scenario, a cube of tightly packed particles without

(a) State at $t = 0$ (b) State at $t = 10000$ (c) State at $t = 50000$

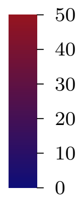

Figure 4.1: Evolution of the simulation state in the equilibrium scenario.

(a) State at $t = 0$ (b) State at $t = 3000$ (c) State at $t = 11000$

(d) State at $t = 22000$ (e) State at $t = 51000$

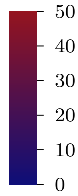

Figure 4.2: Evolution of the simulation state in the exploding liquid scenario.

(a) State at $t = 0$ (b) State at $t = 4000$ (c) State at $t = 12000$

(d) State at $t = 23000$ (e) State at $t = 60000$

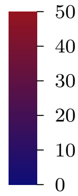

Figure 4.3: Evolution of the simulation state in the heating sphere scenario.

4.1.2 Exploding Liquid

4.1.3 Heating Sphere

4.1.4 Falling Drop

4.1.5 Spinodial Decomposition

4.2 Evaluation Metrics

To compare results between dynamic and static tuning intervals, different metrics can be used. Firstly, the primary goal is to reduce the total simulation runtime for a range of typical scenarios. As tuning phases spend time without advancing the simulation result, a reduction in total runtime is the expected result if our approach reduces the number of tuning phases without spending too many iterations using a suboptimal configuration.

The metric of total runtime is not particularly fine-grained however, as it only takes into account entire simulation runs. To achieve a more detailed benchmark, we also consider the number of iterations that were running on an optimal configuration. As an approximation to the optimal configuration per iteration we use simulation run with static tuning, a high number of tuning samples and a short tuning interval. Based on this static data we can then rank the configuration our dynamic run chose in terms of "optimality".

4.3 Results

4.3.1 Optimality

4.3.2 Runtime

4.3.3 Share of tuning iterations

4.3.4 Trigger Parameters

5 Conclusion

This chapter will ...

5.1 Section 1

5.2 Section 2

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Bibliography

[New+25] Samuel James Newcome et al. "Algorithm Selection in Short-Range Molecular Dynamics Simulations". In: (May 2025). DOI: 10.48550/ARXIV.2505.03438. arXiv: 2505.03438 [cs.CE].

Appendices

A
Showcasing the First Appendix

Writing Guidance

Appendices contain supplementary material **created by the author** that enhances the reader's understanding of the dissertation while not being essential for following the primary narrative. These sections often include detailed tables, figures, complex calculations, or materials like survey questions and interview transcripts produced in the course of the research. The appendices allow readers to explore the research in greater detail, offering a deeper insight into methods and findings without interrupting the main body of work.

B
Showcasing the Second Appendix

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language. Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language. Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language. Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language. Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

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Annexes

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L
Showcasing the First Annex

Writing Guidance

Annexes are supplementary sections in a dissertation that provide additional information or external documents not essential to the main arguments but that support or complement the research. Unlike appendices, **annexes generally contain material that was not developed by the author**, such as reports, legal documents, or published datasets from external sources. This information is placed separately to keep the main content concise, allowing readers access to relevant external references without disrupting the dissertation's flow.