

# <sup>1</sup> ParallelKDE.jl: A Package for Highly Parallel Kernel Density Estimation

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## Software

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## <sup>7</sup> Summary

<sup>8</sup> Kernel density estimation (KDE) is a valuable tool in exploratory analysis, simulation, and probabilistic modeling across the sciences. However, its susceptibility to the curse of dimensionality can make routine KDE prohibitively slow on large, high-dimensional datasets. A central problem in KDE is the choice of the bandwidth of the kernels, which is oftentimes solved by applying an empiric rule-of-thumb (ROT). Furthermore, estimation of non-normal distributions is sometimes approached through non-constant bandwidths—so called adaptive bandwidth—which adds an additional layer of complication. For additional background on KDE and bandwidth selection, see Silverman (1986), Scott (1992), Wand & Jones (1995) and Jones et al. (1996).

<sup>17</sup> ParallelKDE.jl provides a fast, open-source KDE toolkit in Julia (Bezanson et al., 2017) that provides extensible infrastructure to support a variety of methods with serial, multi-threaded and GPU implementations. The package includes (i) a highly parallel implementation of established KDE rules-of-thumb (ROTs) as well as (ii) an implementation of GradePro, a new algorithm described in (Sustay Martinez et al., 2025), engineered here for serial, threaded, and CUDA backends. A lightweight Python wrapper, ParallelKDEPy exposes the same functionality to Python workflows. Our goal is to make robust density estimation practical for large sample sizes of moderate dimensionality through careful parallelization of, mainly, grid-based KDE estimators.

## <sup>26</sup> Statement of need

<sup>27</sup> Many researchers rely on Python implementations of KDE. Popular examples include SciPy's gaussian\_kde (SciPy developers, 2025; Virtanen et al., 2020) with automatic bandwidth selection via ROTs; scikit-learn's KernelDensity (Pedregosa et al., 2011; Scikit-learn developers, 2025), which also supports ROTs; statsmodels' (Seabold & Perktold, 2010) KDEUnivariate and KDEMultivariate estimators with ROTs and cross-validated bandwidths (Statsmodels Developers, 2024); KDEPy's (Odland, 2018) FFTKDE with ROTs and plug-in rules (Sheather & Jones, 1991); and X-Entropy (Kraml et al., 2021), which implements a plug-in rule. While mature and widely used, these tools are CPU-centric and can become slow as data grow in size and dimension, especially if many evaluations are needed in downstream tasks.

<sup>36</sup> ParallelKDE.jl addresses this gap with:

- <sup>37</sup> 1. A unified device interface so that the estimations can be executed on serial, threads (via Julia's Threads.@threads), or GPU (e.g. via CUDA.jl) without changing user code;
- <sup>38</sup> 2. Parallelized calculation of FFT-based KDE with ROTs and GradePro;

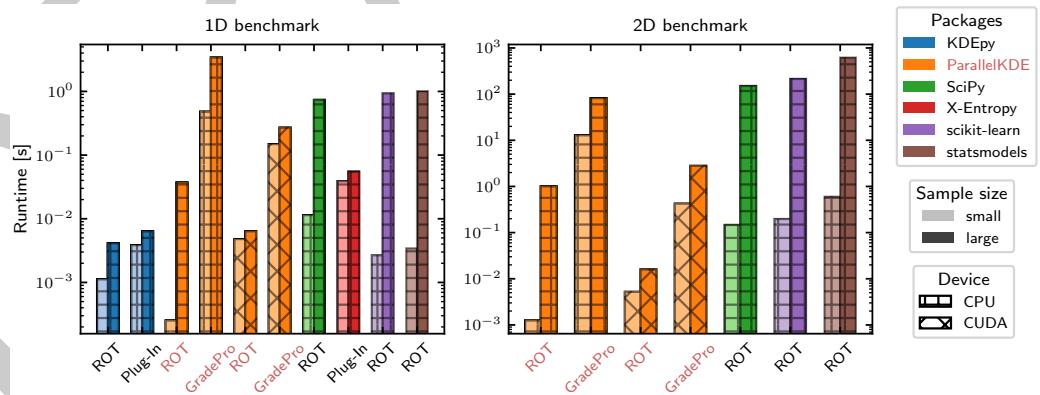
40        3. A reproducible benchmark comparing against SciPy, scikit-learn, statsmodels and KDEpy  
 41        under matched estimation tasks.

## 42        Performance benchmarks

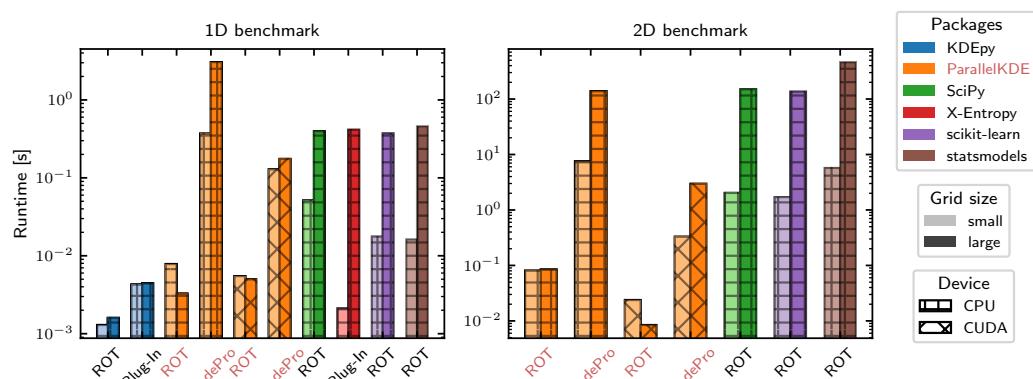
43        To demonstrate that our approach—moving density estimation to parallel execution or parallel  
 44        hardware—produces marked acceleration compared with standard CPU-based libraries, we  
 45        performed an extensive benchmark. We decided to carry it out in Python, since the most  
 46        popular KDE tools are provided for that ecosystem. To ensure consistent interface across  
 47        methods, we ran all experiments through our lightweight wrapper ParallelKDEpy. Naturally,  
 48        our tool can conveniently be used directly in Julia, too. We evaluated different methods on  
 49        synthetic data drawn from 1D and 2D standard normal distributions, generated with SciPy. For  
 50        compatibility with the existing Python tools, we executed CPU baselines single-threaded; in  
 51        addition, we benchmarked our CUDA implementation to exemplify the acceleration achievable  
 52        through parallel execution. To reproduce the benchmark, please refer to the corresponding  
 53        section in the README.md.

54        The results are shown in [Figure 1](#) and [Figure 2](#). Our implementations in ParallelKDE are  
 55        particularly fast for high-resolution grids and/or large datasets. Additionally, our novel method,  
 56        GradePro, achieves high accuracy on diverse distributions. While the CPU version is slower  
 57        than several 1D baselines and comparable in 2D, its performance is still competitive and the  
 58        extra computation yields better accuracy. In CUDA, the method’s parallelism is exposed,  
 59        making it faster and produces superior scaling with problem size. A detailed introduction of  
 60        GradePro along with an extensive investigation of its accuracy is provided in Sustay Martinez  
 61        et al. ([2025](#)).

62        Further comparison of GradePro with other methods is in progress. In the future, we aim  
 63        to provide general recommendations for users on the optimal choice of bandwidth selection  
 64        methods for different use-cases. Here, we focus on the software engineering aspects, which  
 65        enable our fast implementation.



**Figure 1:** Benchmark of common KDE packages and their estimators—rule-of-thumb (ROT), plug-in, and GradePro—along with estimators in ParallelKDE at different sample sizes. The estimations were performed on data drawn from a standard normal distribution. In 1D, 100 and 100,000 samples were used with a grid of 500 points. In 2D, 1,000 and 1,000,000 samples were used with a grid of 100 points per dimension. Reported runtimes are averages over 10 repetitions. Hardware: Intel Core i7-6700 (single-threaded) and NVIDIA GTX 1080.



**Figure 2:** Benchmark of common KDE packages and their estimators along with estimators in ParallelKDE at different grid sizes. The estimations were performed on data drawn from a standard normal distribution. In 1D, 100 and 2,500 grid points were used with 10,000 samples. In 2D, 33 and 300 grid points per dimension were used with 100,000 samples. Reported runtimes are averages over 10 repetitions. Hardware: Intel Core i7-6700 (single-threaded) and NVIDIA GTX 1080.

## 66     **Functionality**

67     **Design and architecture.** ParallelKDE.jl is organized around a minimal device interface that  
68     isolates parallelism from algorithmic logic. We ship three backends:

- 69       ■ Serial CPU for portability and determinism;
- 70       ■ Threaded CPU using Julia’s built-in multithreading;
- 71       ■ CUDA GPU via CUDA.jl (Besard, Foket, et al., 2019; Besard, Churavy, et al., 2019).

72     **Implemented methods.** The package includes (a) KDE with parallel ROTs, namely Scott  
73     and Silverman, for rapid baselines and (b) GradePro, engineered to perform rapid adaptive  
74     KDE in multiple dimensions. This implementation effectively performs independent grid-point-  
75     wise density estimation using FFT (Frigo & Johnson, 2005). Throughout the routines, the  
76     necessary memory is reduced by reusing allocated memory, without damaging performance.  
77     The serial version serves as a reference; the threaded version parallelizes routines applied over  
78     the bootstrap re-samples (which are required by the method); the CUDA routines provide  
79     parallelization at each estimated grid-point. Each implemented method naturally exposes all  
80     its parameters up to the user. Convenient defaults are set where reasonable. Figure 3 shows a  
81     flowchart of the implemented algorithm.

82     **Reproducibility and testing.** We include timing benchmarks to illustrate the speed gains  
83     obtained from parallelizable KDE algorithms.

84     **Python wrapper.** The companion package ParallelKDEPy provides, with the help of  
85     PythonCall.jl (Rowley, 2022), Python bindings to ParallelKDE.jl, offering identical  
86     estimators and device selection for seamless integration in Python-based workflows.

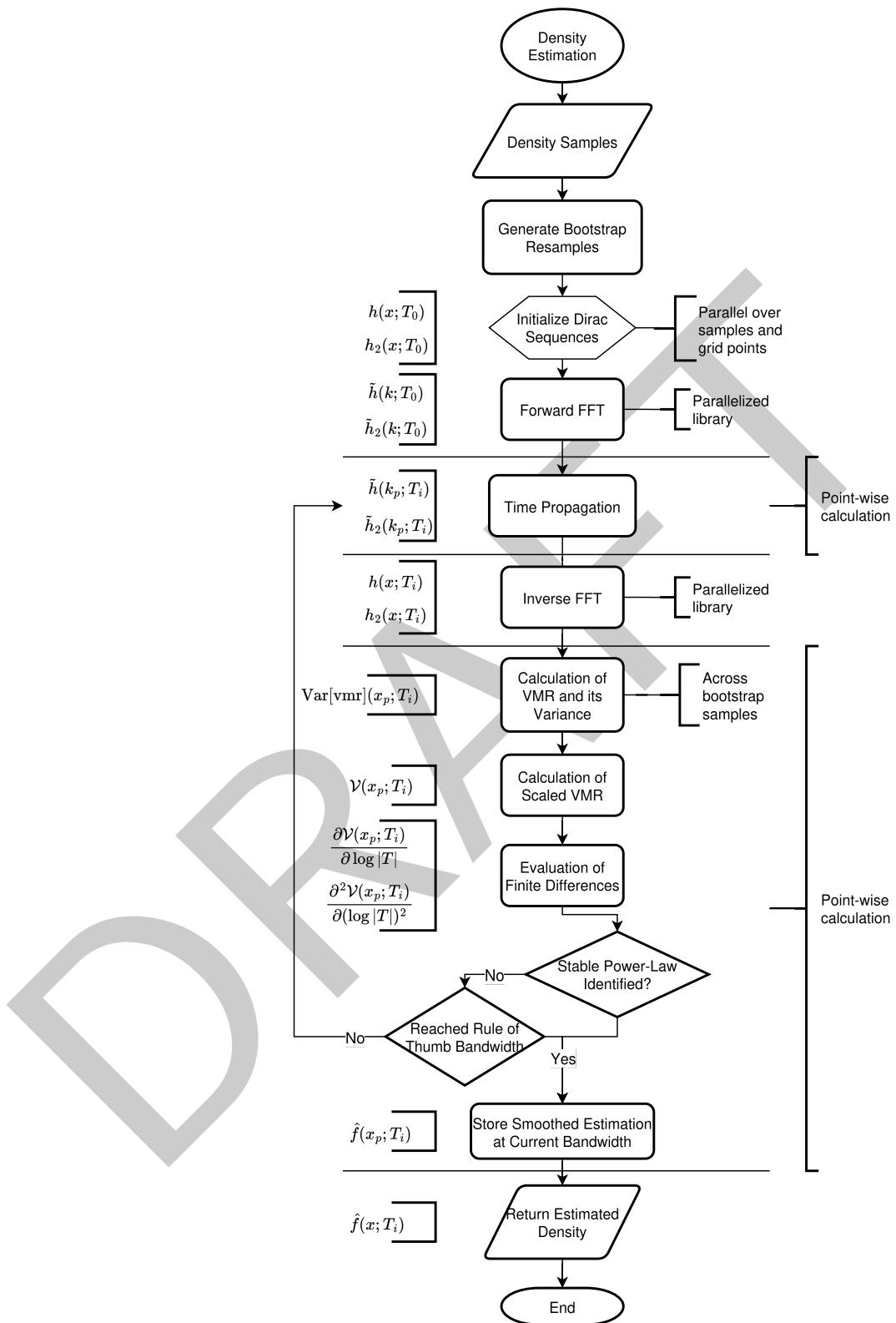


Figure 3: Flowchart of the parallelizable point-wise density estimation algorithm.

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## 90 References

- 91 Besard, T., Churavy, V., Edelman, A., & Sutter, B. D. (2019). Rapid software prototyping for  
92 heterogeneous and distributed platforms. *Advances in Engineering Software*, 132, 29–46.  
93 <https://doi.org/10.1016/j.advengsoft.2019.02.002>
- 94 Besard, T., Foket, C., & De Sutter, B. (2019). Effective Extensible Programming: Unleashing  
95 Julia on GPUs. *IEEE Transactions on Parallel and Distributed Systems*, 30(4), 827–841.  
96 <https://doi.org/10.1109/tpds.2018.2872064>
- 97 Bezanson, J., Edelman, A., Karpinski, S., & Shah, V. B. (2017). Julia: A Fresh Approach to  
98 Numerical Computing. *SIAM Review*, 59(1), 65–98. <https://doi.org/10.1137/141000671>
- 99 Frigo, M., & Johnson, S. G. (2005). The Design and Implementation of FFTW3. *Proceedings  
100 of the IEEE*, 93(2), 216–231. <https://doi.org/10.1109/JPROC.2004.840301>
- 101 Jones, M. C., Marron, J. S., & Sheather, S. J. (1996). A Brief Survey of Bandwidth Selection  
102 for Density Estimation. *Journal of the American Statistical Association*, 91(433), 401–407.  
103 <https://doi.org/10.1080/01621459.1996.10476701>
- 104 Kraml, J., Hofer, F., Quoika, P. K., Kamenik, A. S., & Liedl, K. R. (2021). X-Entropy: A  
105 Parallelized Kernel Density Estimator with Automated Bandwidth Selection to Calculate  
106 Entropy. *Journal of Chemical Information and Modeling*, 61(4), 1533–1538. <https://doi.org/10.1021/acs.jcim.0c01375>
- 108 Odland, T. (2018). *Tommyod/KDEpy: Kernel Density Estimation in Python*. <https://doi.org/10.5281/ZENODO.2392268>
- 110 Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., Blondel,  
111 M., Prettenhofer, P., Weiss, R., Dubourg, V., Vanderplas, J., Passos, A., Cournapeau,  
112 D., Brucher, M., Perrot, M., & Duchesnay, É. (2011). Scikit-learn: Machine Learning  
113 in Python. *Journal of Machine Learning Research*, 12(85), 2825–2830. <http://jmlr.org/papers/v12/pedregosa11a.html>
- 115 Rowley, C. (2022). *PythonCall.jl: Python and Julia in harmony*. <https://github.com/JuliaPy/PythonCall.jl>
- 117 Scikit-learn developers. (2025). *KernelDensity - scikit-learn 1.7.2 Documentation*.  
118 <https://scikit-learn.org/stable/modules/generated/sklearn.neighbors.KernelDensity.html#sklearn.neighbors.KernelDensity>
- 120 SciPy developers. (2025). *Scipy.stats.gaussian\_kde - SciPy v1.16.2 Documentation*. [https://docs.scipy.org/doc/scipy/reference/generated/scipy.stats.gaussian\\_kde.html](https://docs.scipy.org/doc/scipy/reference/generated/scipy.stats.gaussian_kde.html)
- 122 Scott, D. W. (1992). *Multivariate Density Estimation: Theory, Practice, and Visualization*  
123 (1st ed.). Wiley. <https://doi.org/10.1002/9780470316849>
- 124 Seabold, S., & Perktold, J. (2010). Statsmodels: Econometric and statistical modeling with  
125 python. *Proceedings of the 9th Python in Science Conference*. <https://doi.org/10.25080/majora-92bf1922-011>
- 127 Sheather, S. J., & Jones, M. C. (1991). A Reliable Data-Based Bandwidth Selection Method  
128 for Kernel Density Estimation. *Journal of the Royal Statistical Society Series B: Statistical  
129 Methodology*, 53(3), 683–690. <https://doi.org/10.1111/j.2517-6161.1991.tb01857.x>
- 130 Silverman, B. W. (1986). *Density estimation for statistics and data analysis*. Chapman; Hall.

- 131 ISBN: 978-0-412-24620-3
- 132 Statsmodels Developers. (2024). *Statsmodels v0.14.4 Documentation*. [https://www.statsmodels.org/stable/generated/statsmodels.nonparametric.kernel\\_density.KDEMultivariate.html](https://www.statsmodels.org/stable/generated/statsmodels.nonparametric.kernel_density.KDEMultivariate.html)
- 133  
134
- 135 Sustay Martinez, C., Quoika, P. K., & Zacharias, M. (2025). Novel Rapid Approach for  
136 Adaptive Gaussian Kernel Density Estimation: Gridpoint-wise Propagation of Anisotropic  
137 Diffusion Equation. *Researchsquare*. <https://doi.org/10.21203/rs.3.rs-8038701/v1>
- 138 Virtanen, P., Gommers, R., Oliphant, T. E., Haberland, M., Reddy, T., Cournapeau, D.,  
139 Burovski, E., Peterson, P., Weckesser, W., Bright, J., Van Der Walt, S. J., Brett, M.,  
140 Wilson, J., Millman, K. J., Mayorov, N., Nelson, A. R. J., Jones, E., Kern, R., Larson, E.,  
141 ... Vázquez-Baeza, Y. (2020). SciPy 1.0: Fundamental algorithms for scientific computing  
142 in Python. *Nature Methods*, 17(3), 261–272. <https://doi.org/10.1038/s41592-019-0686-2>
- 143 Wand, M. P., & Jones, M. C. (1995). *Kernel smoothing* (1. ed). Chapman & Hall. ISBN: 978-  
144 0-429-17059-1

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