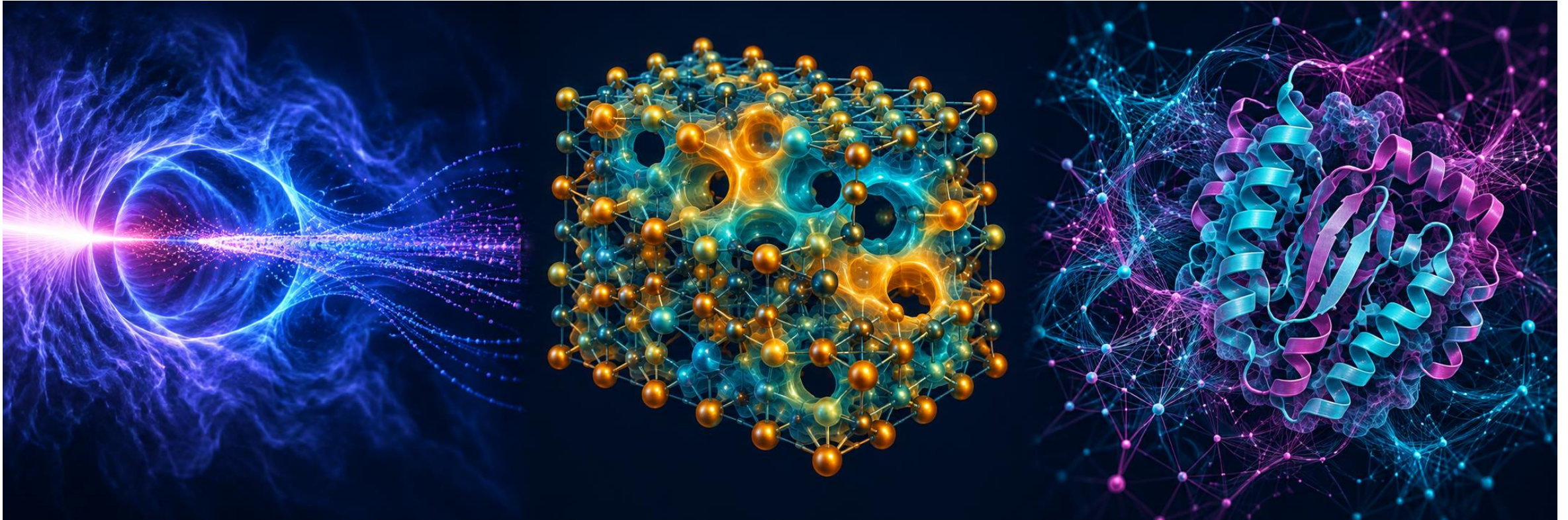


Kolotinskii D.A., Timofeev A.V.

Application of GPUs to Non-Equilibrium Plasma Simulation

Where GPUs deliver scientific results



PLASMA PHYSICS

Particle-in-cell simulation

PIConGPU: particles and electromagnetic fields

MATERIALS DESIGN

Atomistic molecular dynamics

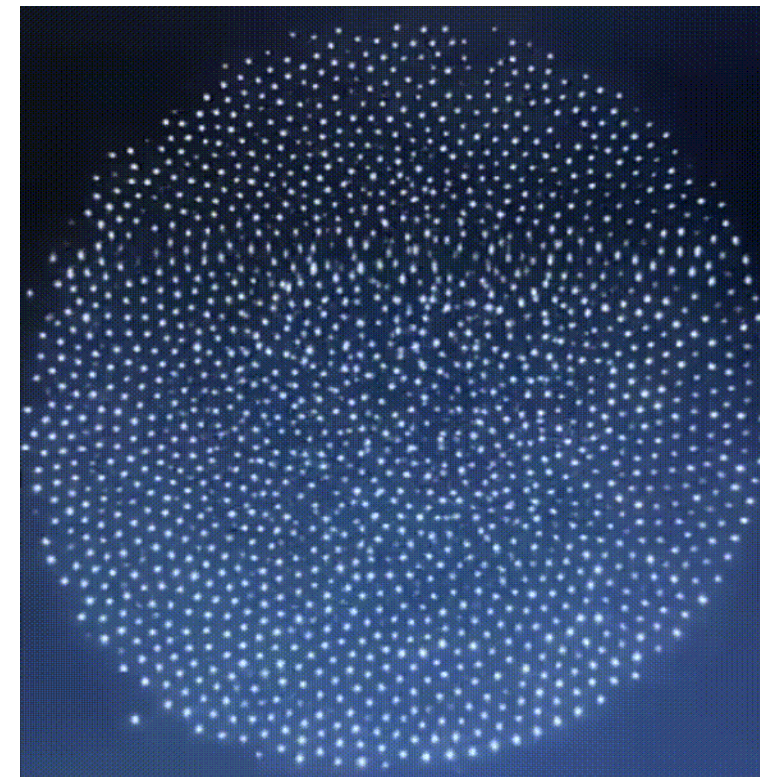
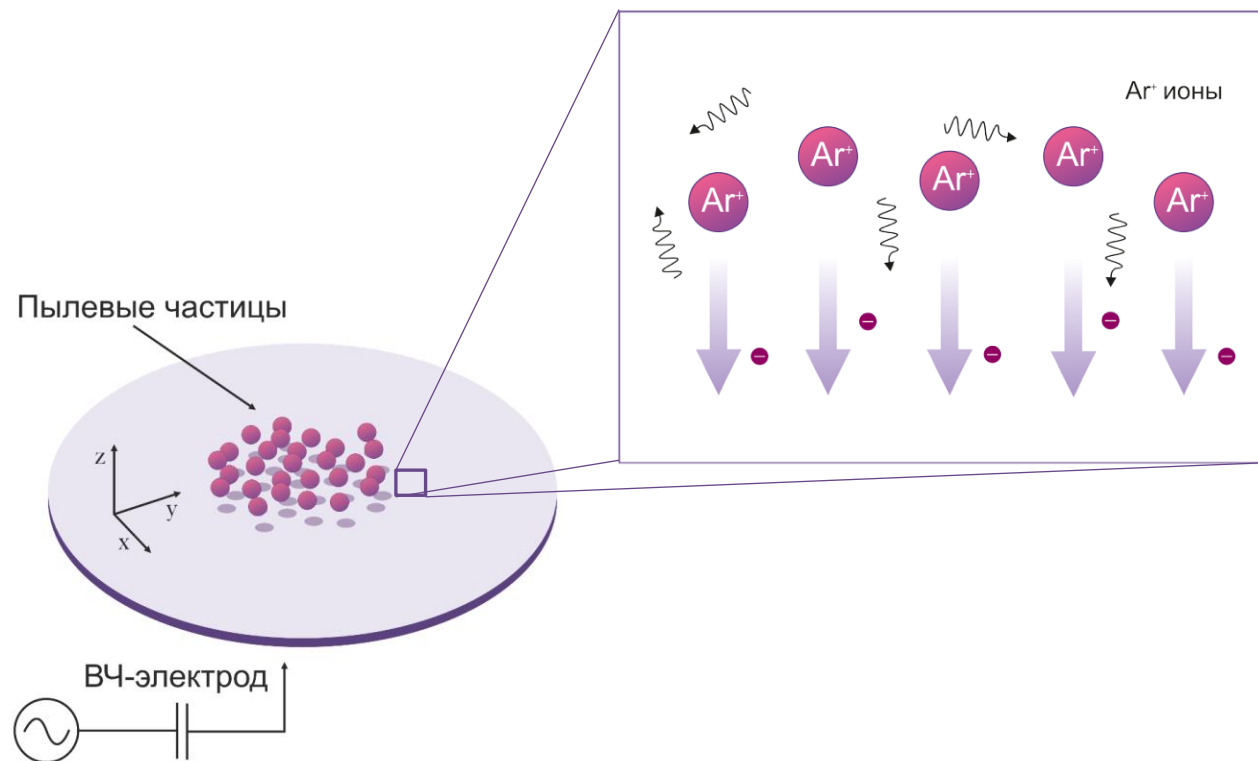
EXAALT: interatomic forces and long-time evolution

SCIENTIFIC AI

Molecular structure prediction

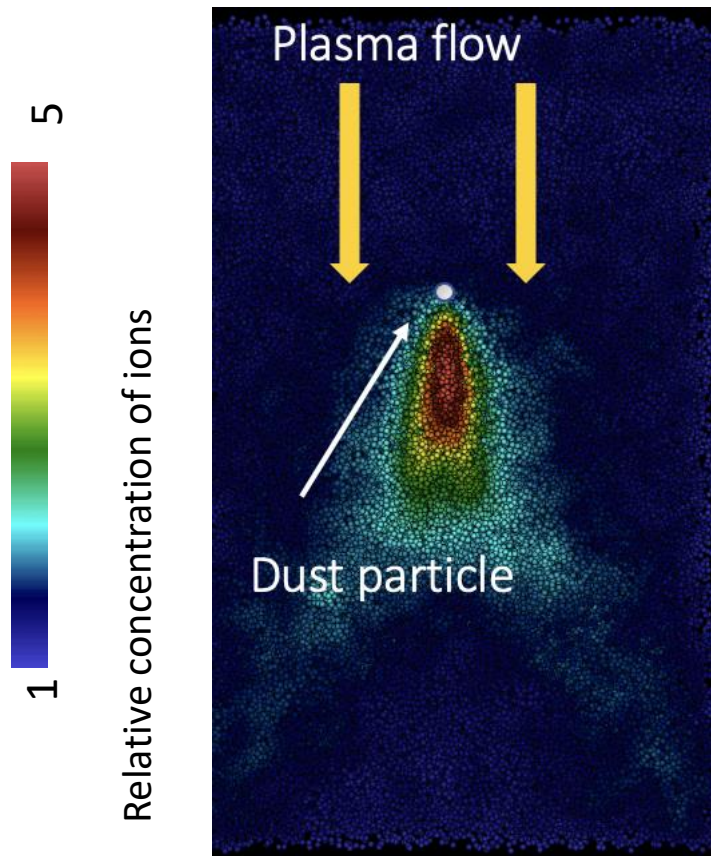
AlphaFold: GPU inference on protein structures

Dusty plasmas



Hariprasad M. G.,..., V.S. Nikolaev, D.A.Kolotinskii, A.V.Timofeev
//Scientific Reports. – 2022. – Т. 12. – №. 1. – С. 13882.

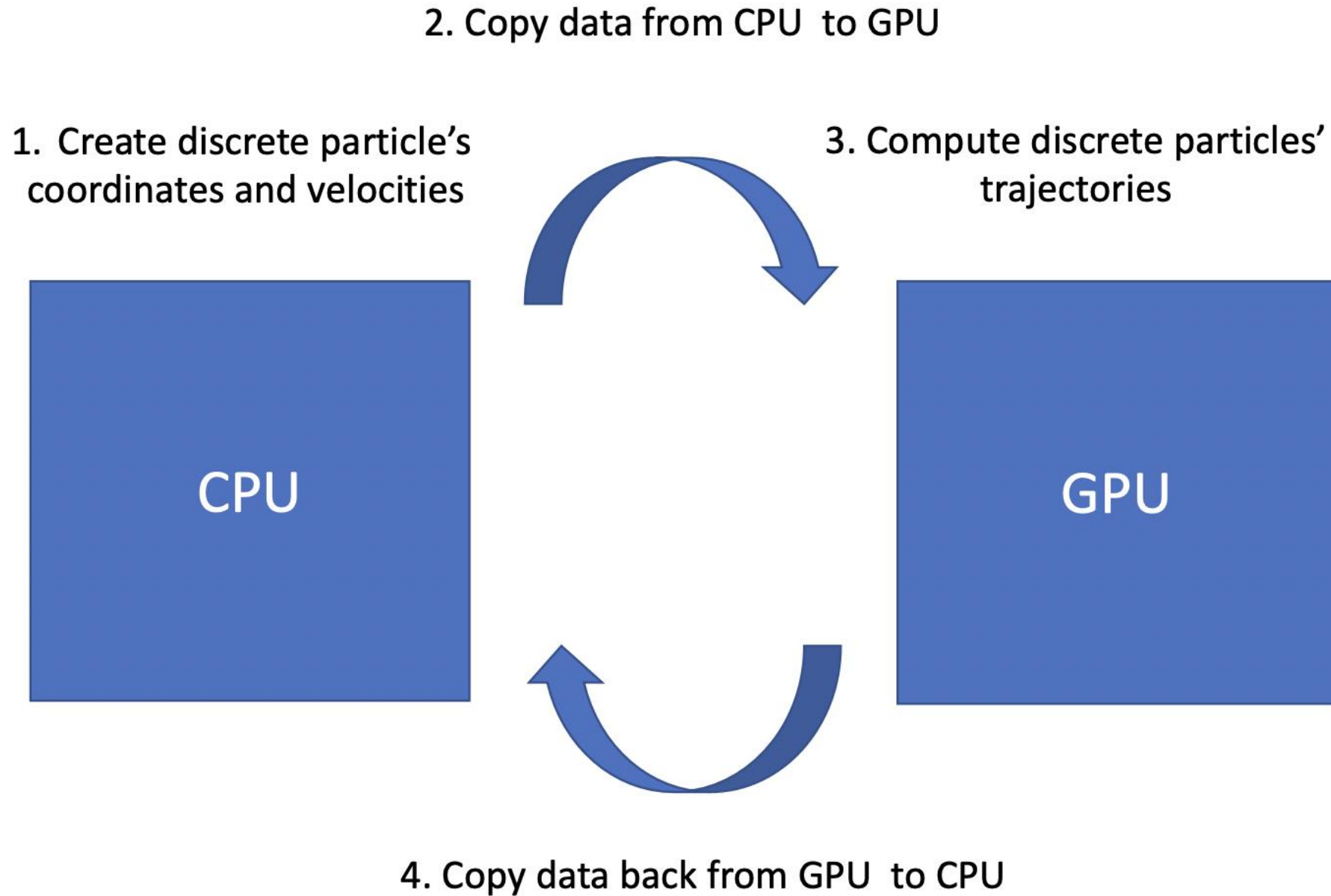
The bottleneck of dusty plasmas simulation



$$\mathbf{F}_{ij} = \frac{q_i q_j}{4\pi\epsilon_0} \frac{1 + |\mathbf{r}_i - \mathbf{r}_j|/r_{De}}{|\mathbf{r}_i - \mathbf{r}_j|^3} \exp\left(-\frac{|\mathbf{r}_i - \mathbf{r}_j|}{r_{De}}\right) (\mathbf{r}_j - \mathbf{r}_i)$$

D. A. Kolotinskii, A. V. Timofeev // Computer Physics Communications. — 2023.

D. A. Kolotinskii, A. V. Timofeev // Lecture Notes in Computer Science, 2022. – C. 276-289.



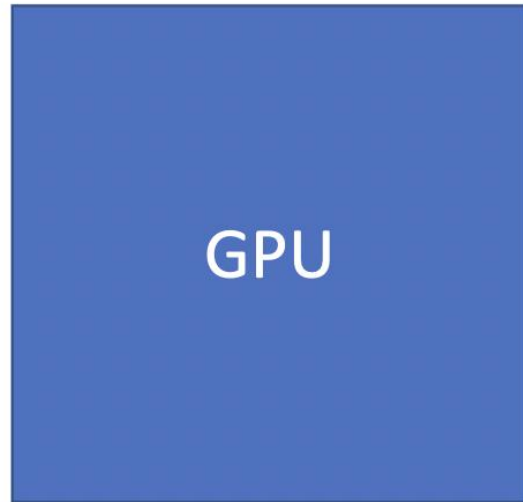
1. Scatter discrete particles' positions



2. Gather partial forces



3. Compute partial forces



4. Sum all partial forces
in a single GPU

3. Compute partial forces



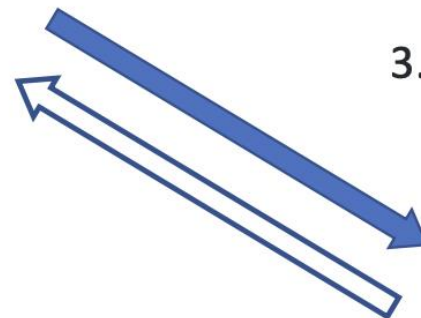
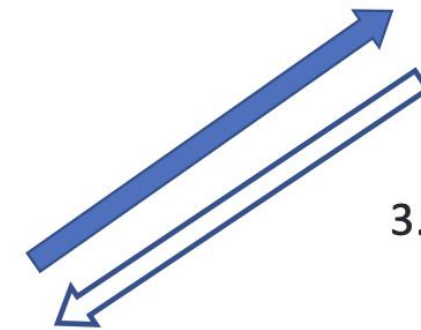
3. Compute partial forces



3. Compute partial forces



3. Compute partial forces



Solution

Which devices we study?

Device	Peak performance (TFLOPS)	Energy consumption (Watt)	Price (\$)
NVIDIA A30	10.32	165	5000
NVIDIA A100	19.5	400	31000
NVIDIA V100	15.7	300	13000
Intel Xeon Gold	10	140	3600

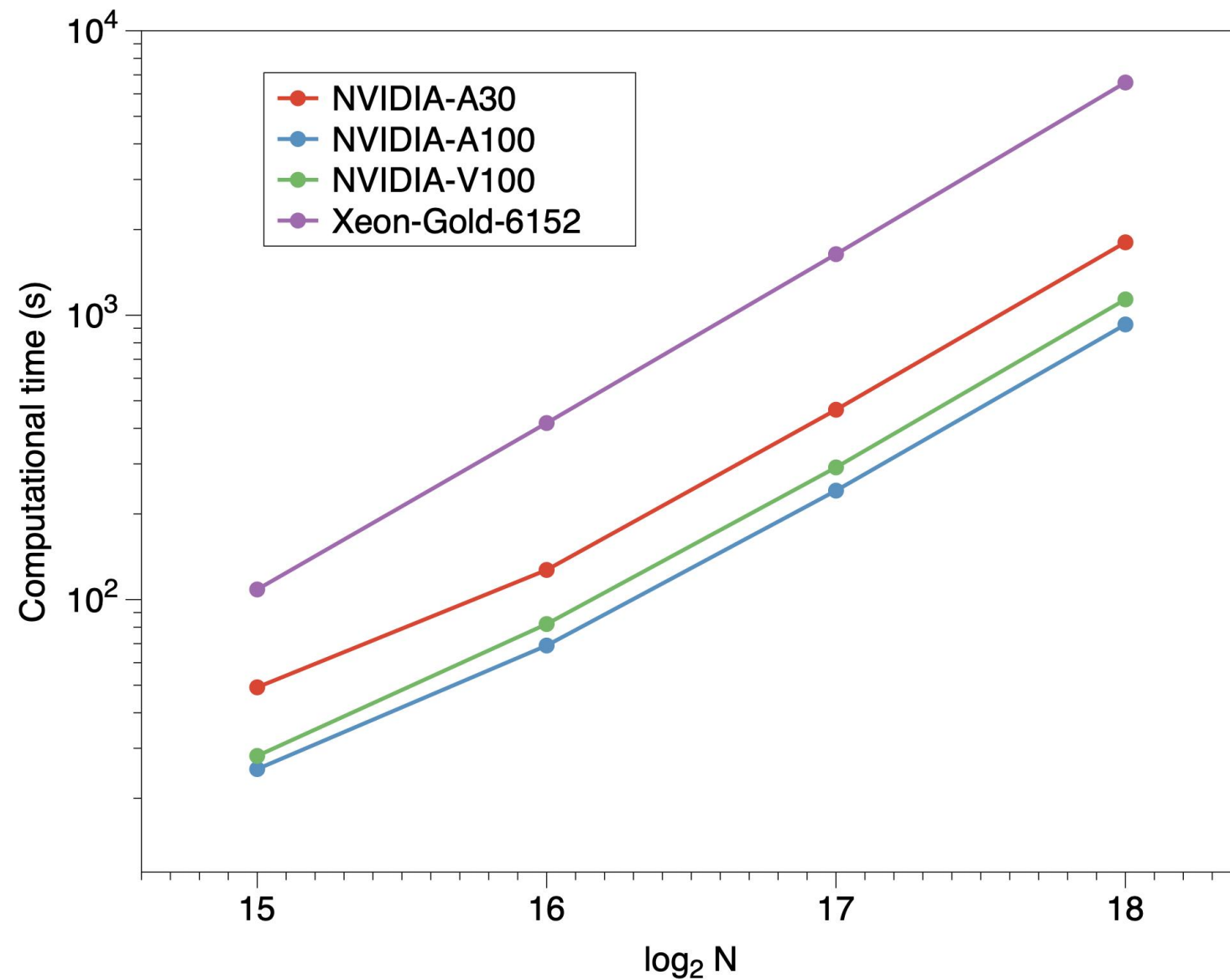
Which metrics we study for a given test case?

Resource efficiency: Normalized $\frac{\text{number of interactions}}{\text{second}}$ per peak performance

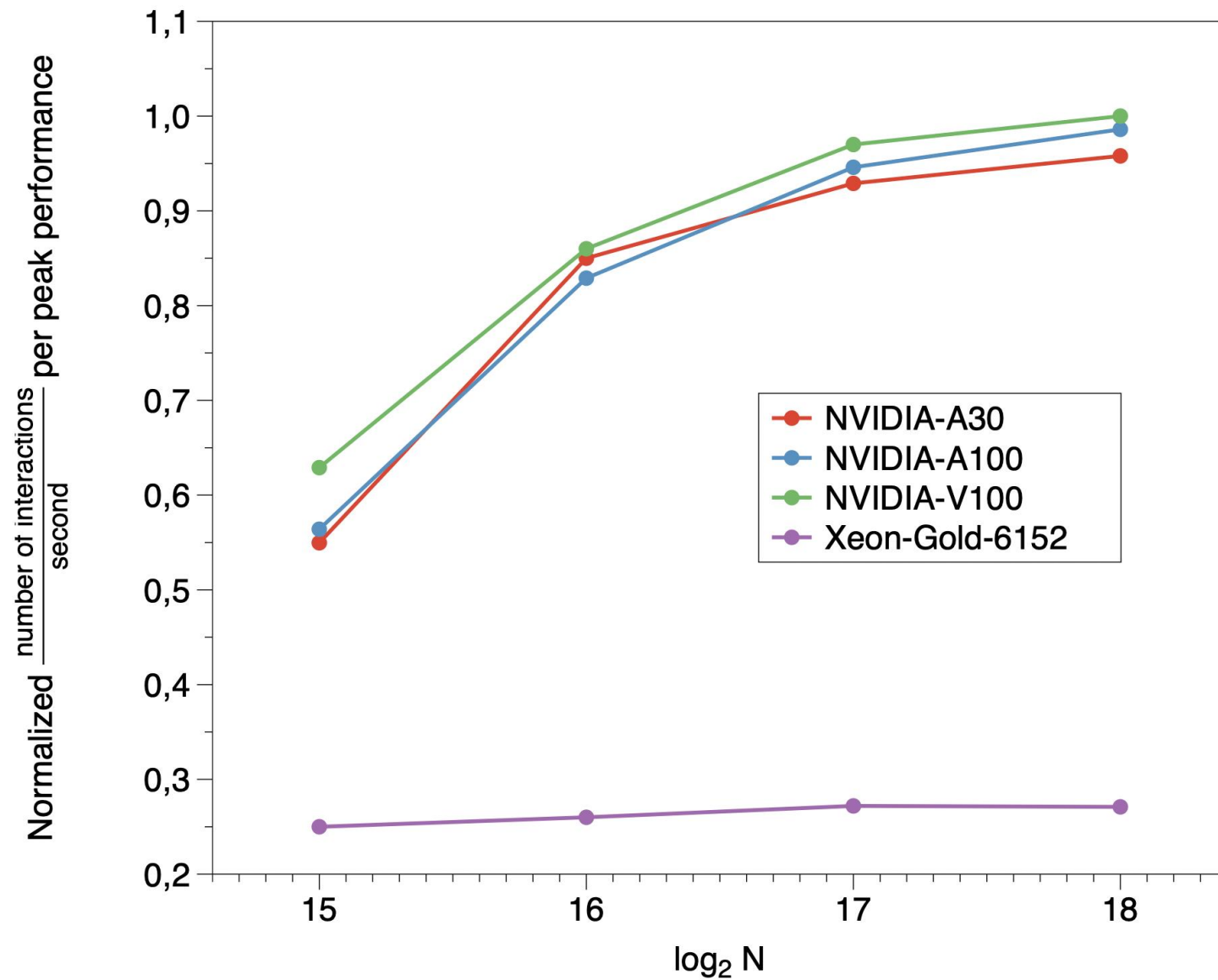
Economical efficiency: $\frac{\text{Number of interactions}}{\text{second}}$ per dollar

Power efficiency: $\frac{\text{Number of interactions}}{\text{second}}$ per Watt

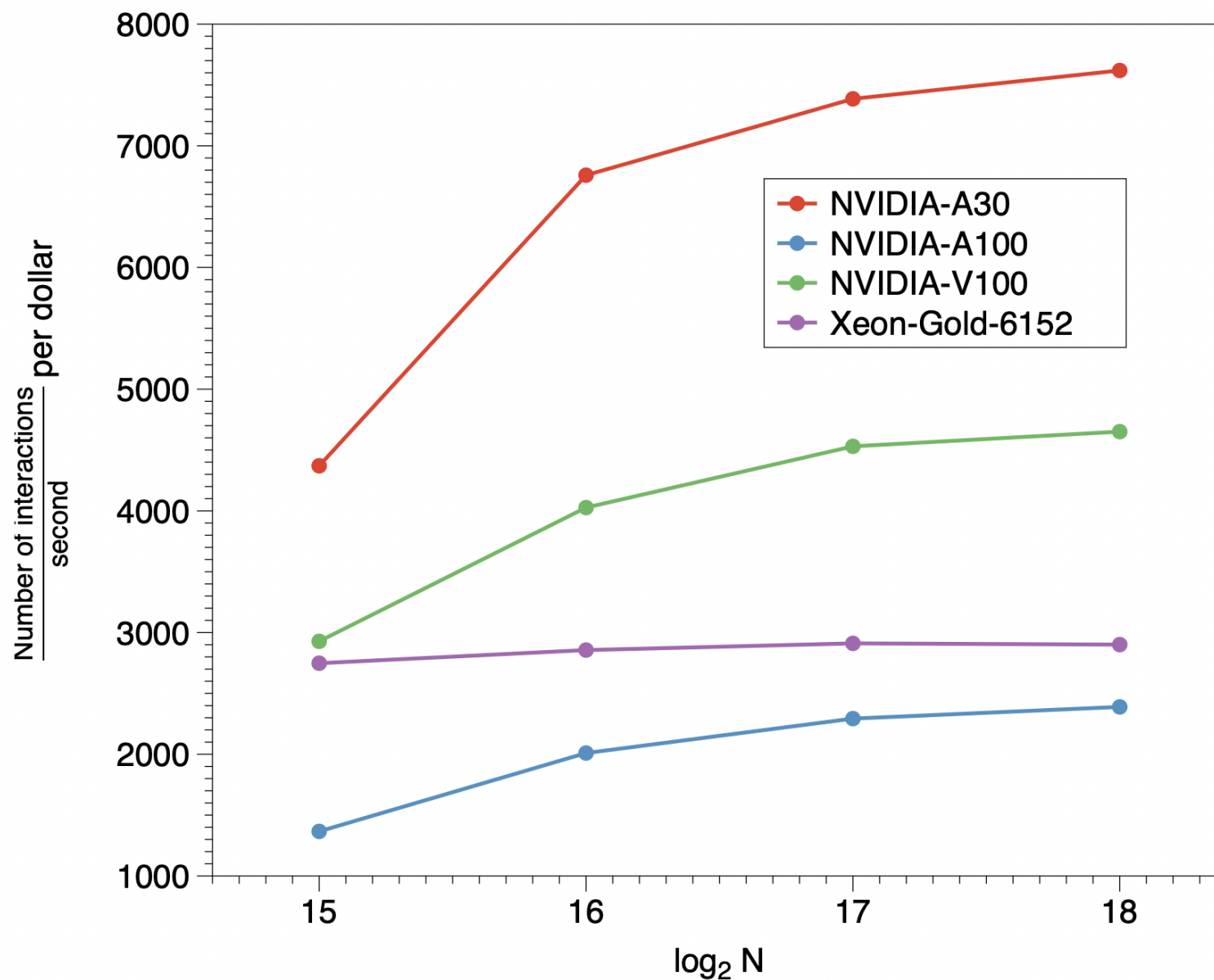
Computational time



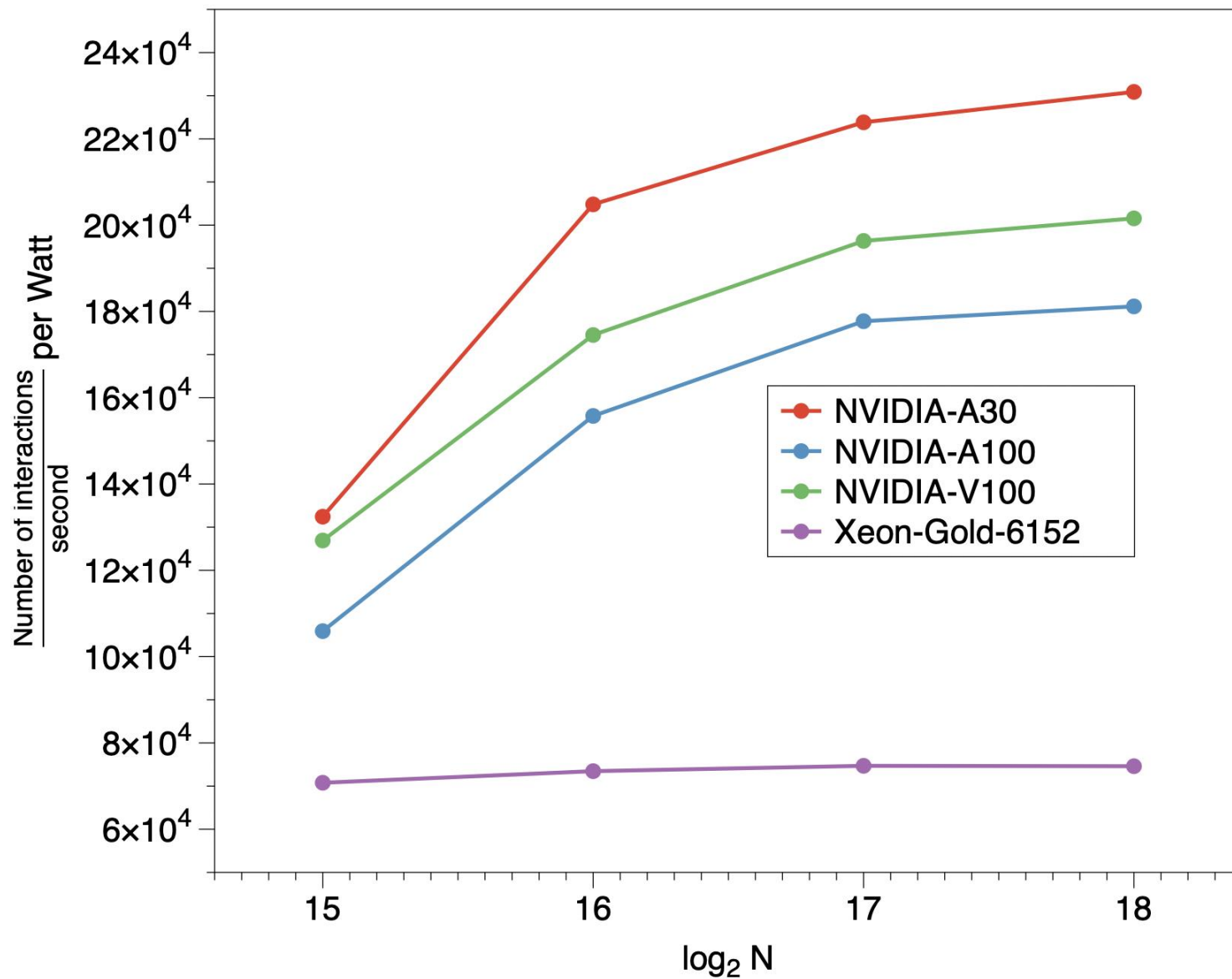
Resource efficiency



Economical efficiency



Power efficiency

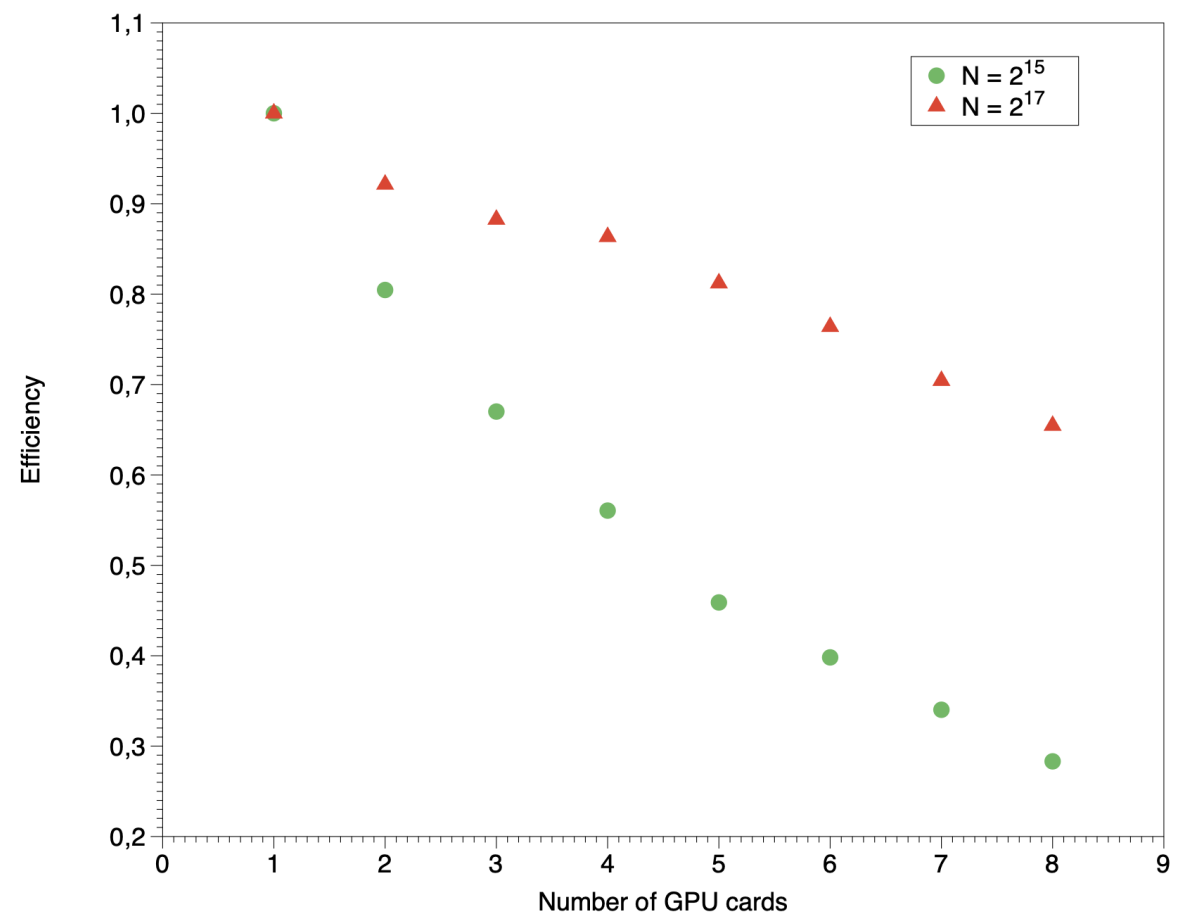
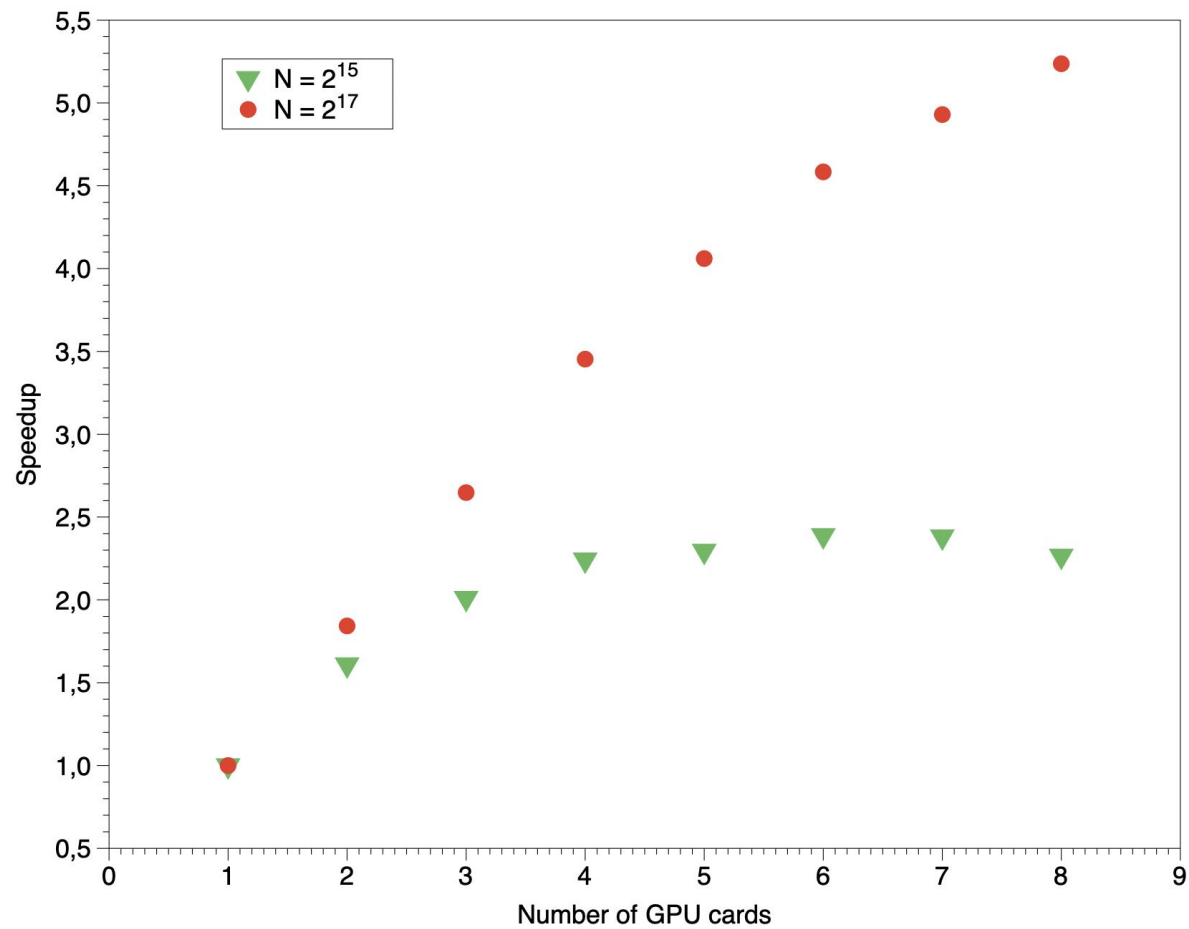


Device ranking

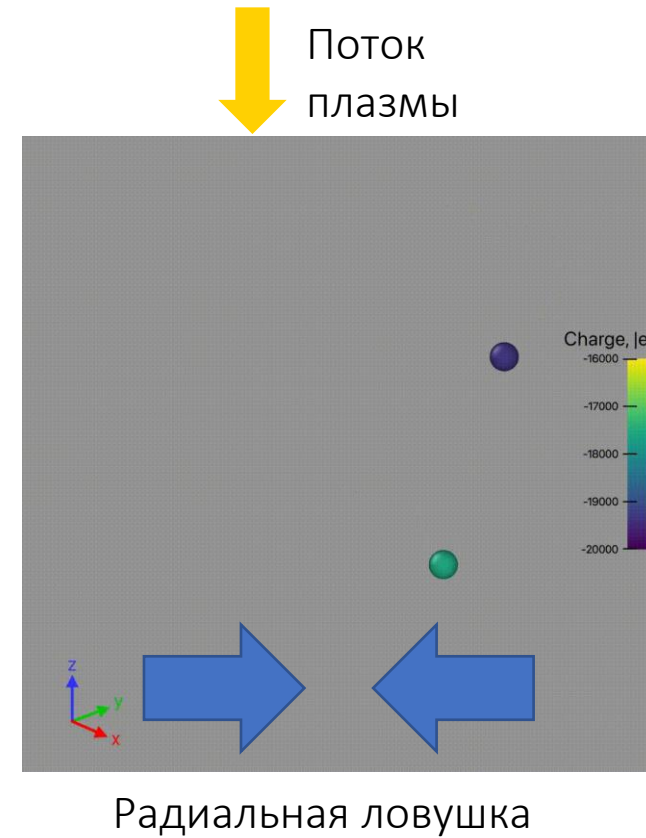
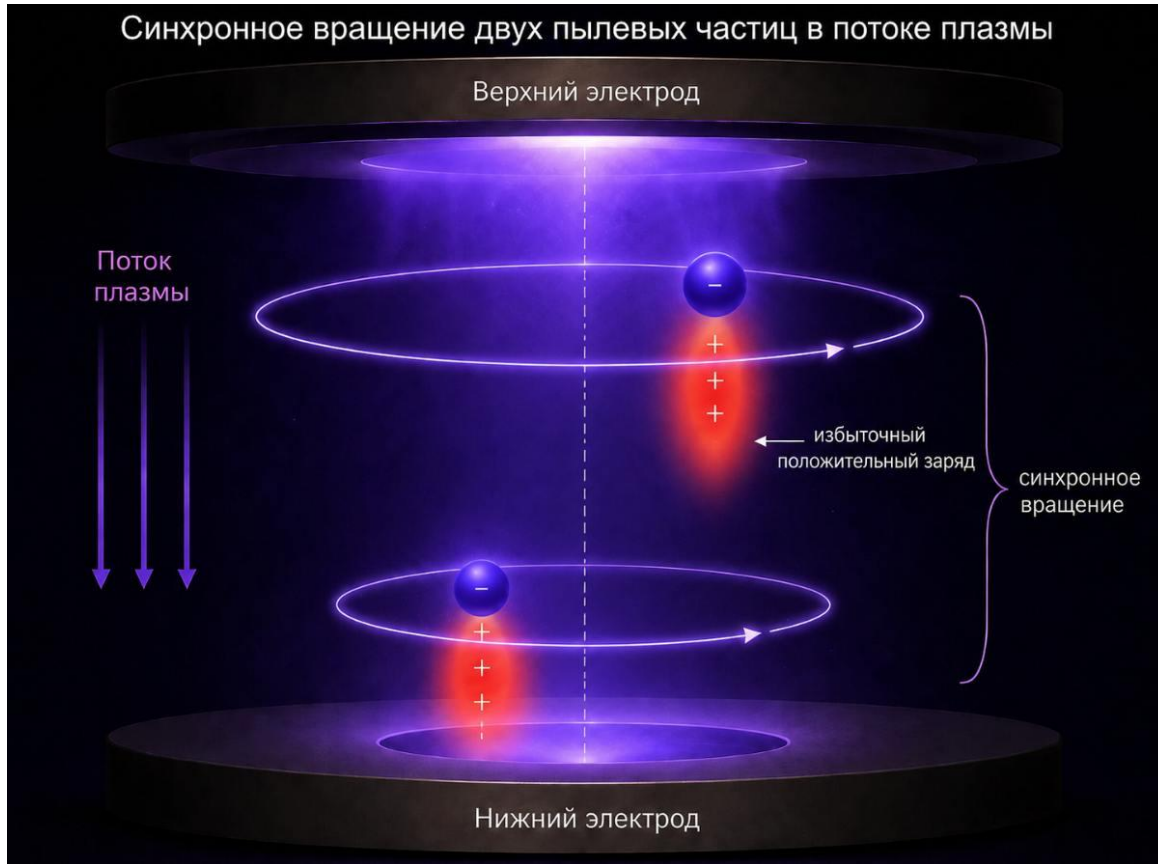
Metric/Device	NVIDIA A30	NVIDIA A100	NVIDIA V100	Intel Xeon Gold
Computational time	3	1	2	4
Resource efficiency	2	2	1	3
Economical efficiency	1	4	2	3
Power efficiency	1	3	2	4

1. NVIDIA V100 (7 points and no > 2)
2. NVIDIA A30 (7 points)
3. NVIDIA A100 (10 points)
4. Intel Xeon Gold (14)

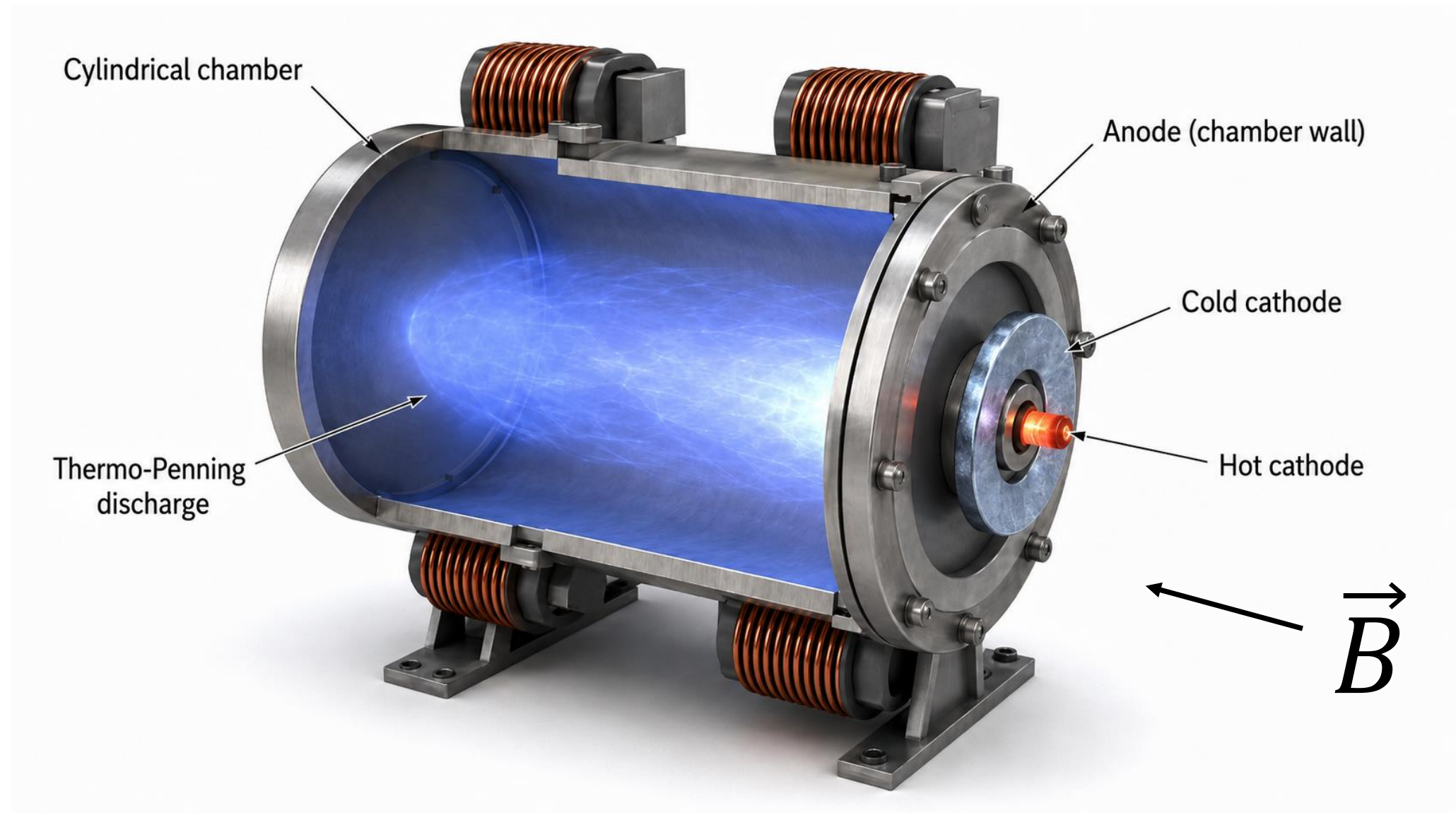
Usage of several GPUs



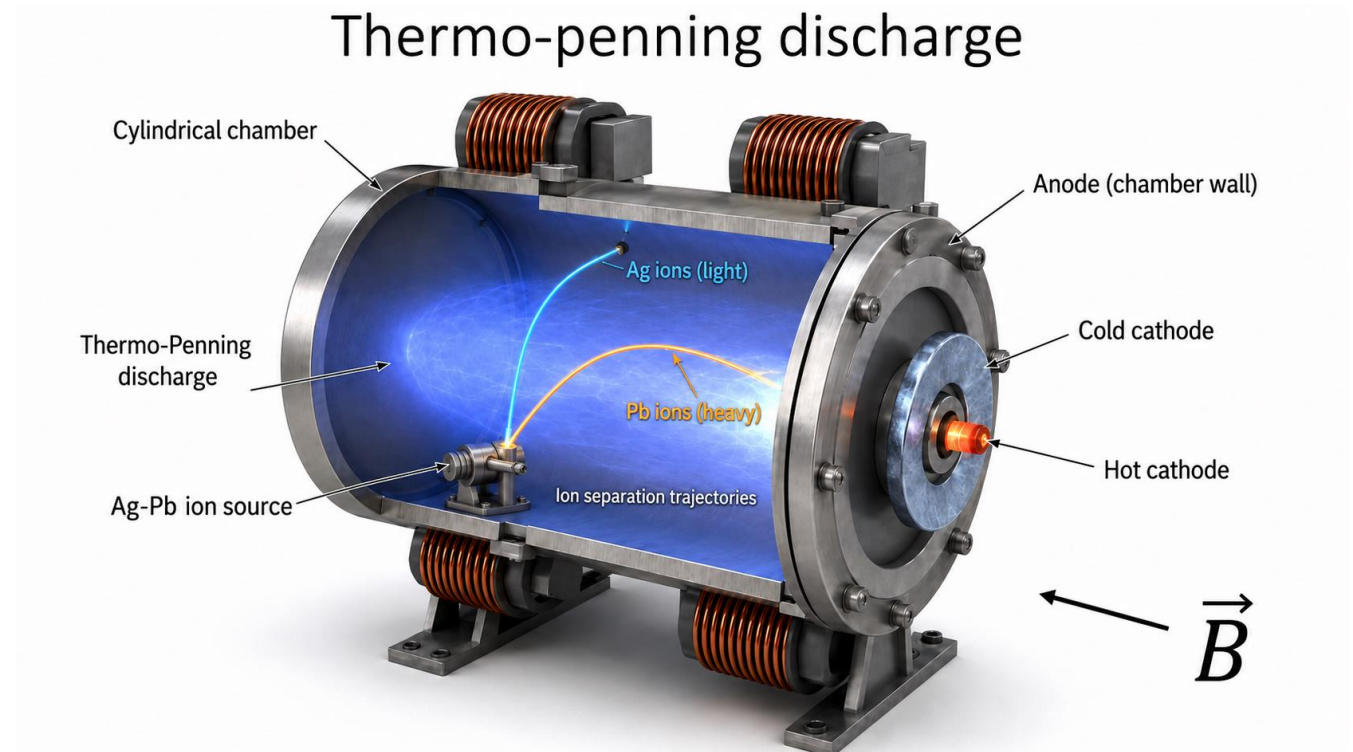
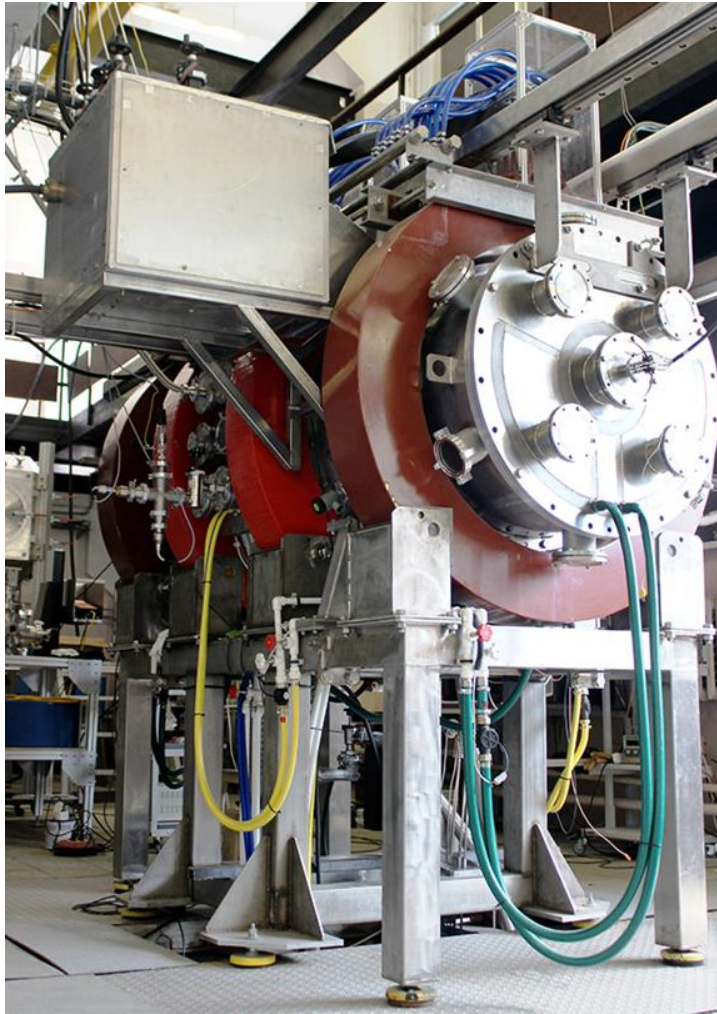
Enabling multiscale simulation of dusty plasmas



Thermo-penning discharge

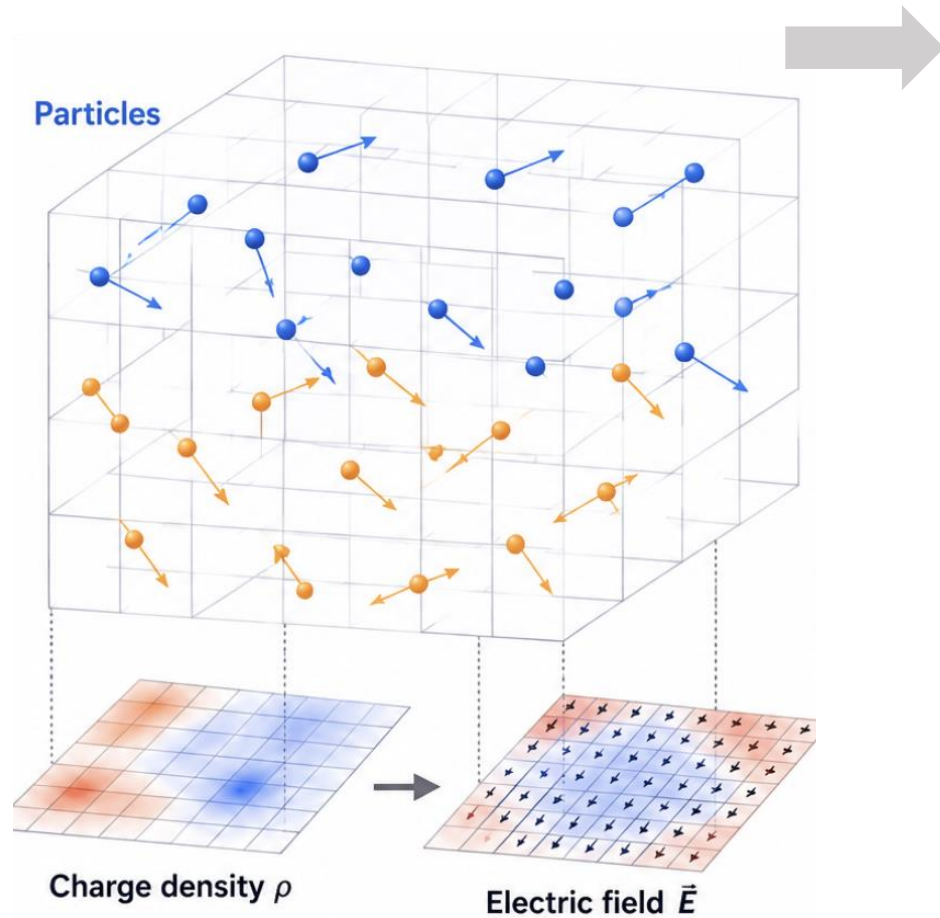


Plasma based nuclear waste separation technology



N.A. Vorona, A.V. Gavrikov, A.A. Samokhin, V.P. Smirnov, Yu.S. Khomyakov, 2014, published in Yadernaya Fizika i Inzhiniring, 2014, Vol. 5, Nos. 11–12, pp. 944–951.

Porting Particle-In-Cell on GPU with JAX

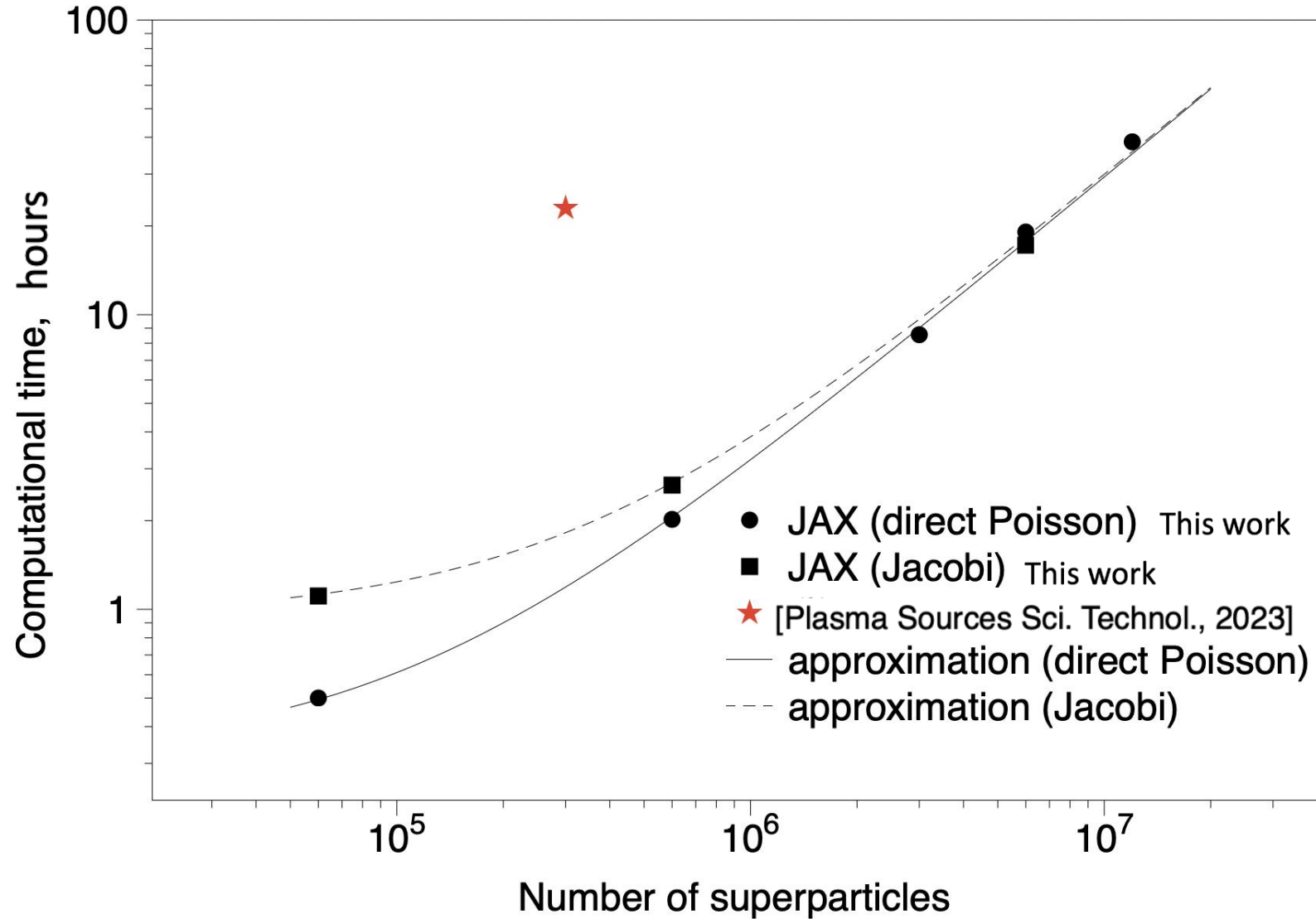


High performance array computing

JAX is a Python library for accelerator-oriented array computation and program transformation, designed for high-performance numerical computing and large-scale machine learning.



Performance comparison



Multiscale simulation of plasma based separation

гирокинетика электронов → ионы и нейтралы (GPU, PIC/MCC) → редуцированная модель плазмы → разделение ионов

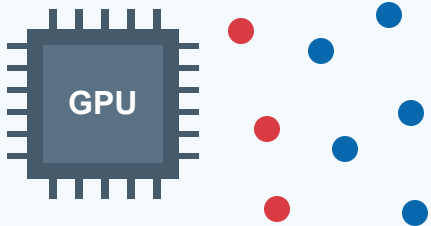
1 Электроны

Гирокинетическое описание
электронной компоненты в
магнитном поле



2 Ионы и нейтралы плазмы

GPU-ускоренный
PIC/MCC, JAX,
миллионы суперчастиц

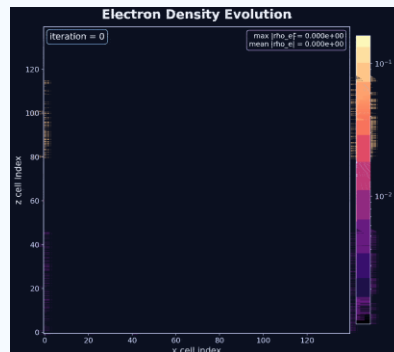


3 Прямое моделирование плазмы разряда Пеннинга



- Потенциал
- Плотности
- Неустойчивости

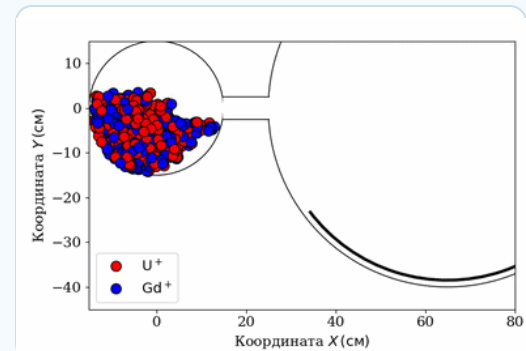
Эволюция распределения плазмы



4 Переход на следующий масштаб

- Аппроксимация характеристик плазмы, неустойчивости и параметров флуктуаций из дорогих прямых расчётов
- Редуцированная модель (самосогласованные поля, флуктуации, неустойчивости)
- Сохранение ключевой физики

5 Траектории разделяемых ионов в редуцированной модели плазмы



**Качественное
разделение ионов**
селективность, ширина зон
осаждения, чистота

Conclusions

GPUs can be efficiently used to accelerate simulation of complex plasmas for fundamental and applied research

