Toward efficient GPU-accelerated *N*-body simulations

Mark J. Stock, Ph.D. and Adrin Gharakhani, Sc.D.

Applied Scientific Research
Santa Ana, CA

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Definitions

- GPU - Graphics Processing Unit
- GPGPU - General-Purpose programming for GPUs
- Flop - Floating point operation
- GFlop/s - Billion Flops per second

Two Nvidia 9800GX2 GPUs
> 1 TFlop/s

[Tom's Hardware]

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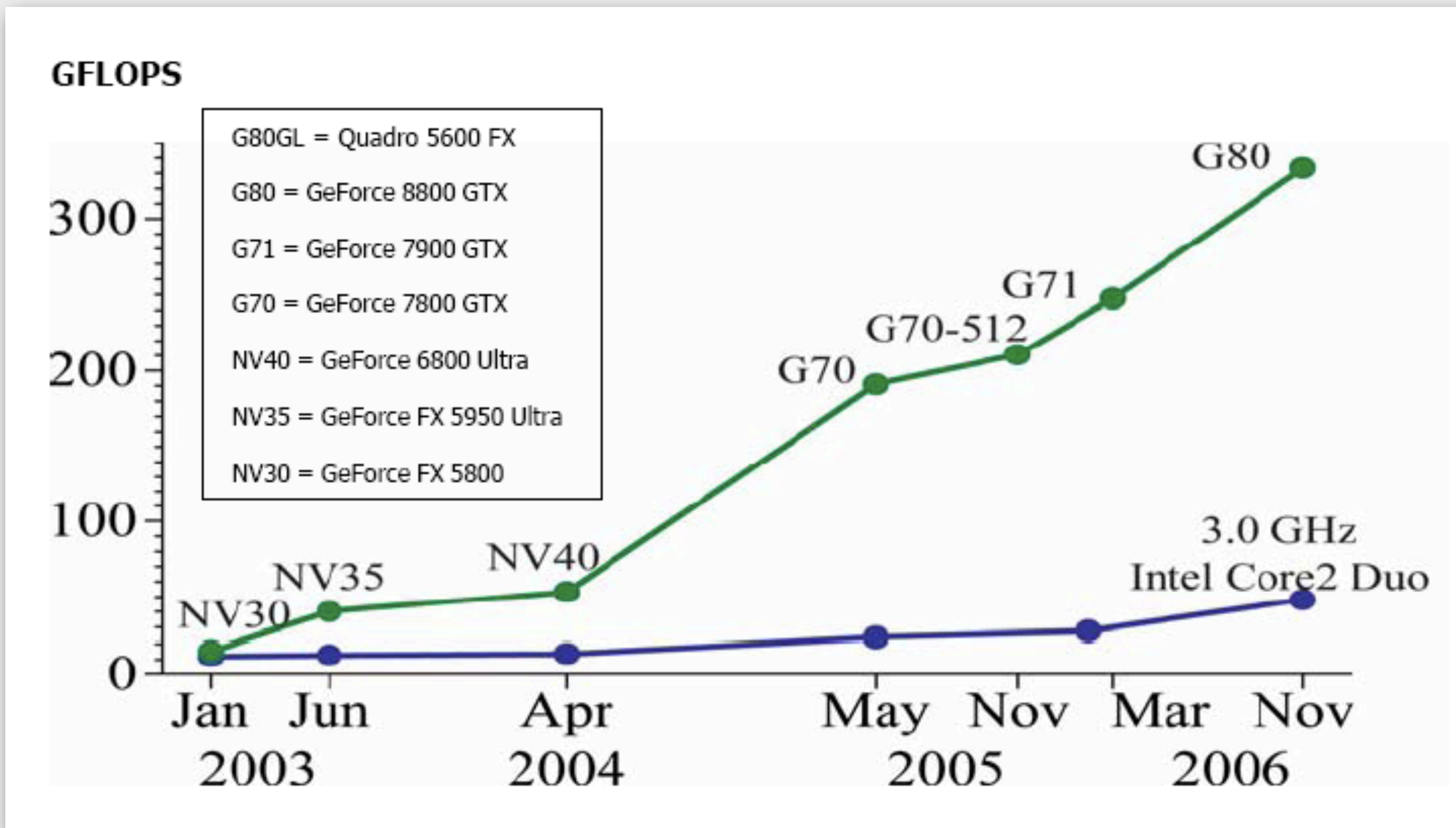
Motivation

- GPU performance doubles ~1 year
- CPU performance doubles ~2 years



NVIDIA CUDA Programming Guide

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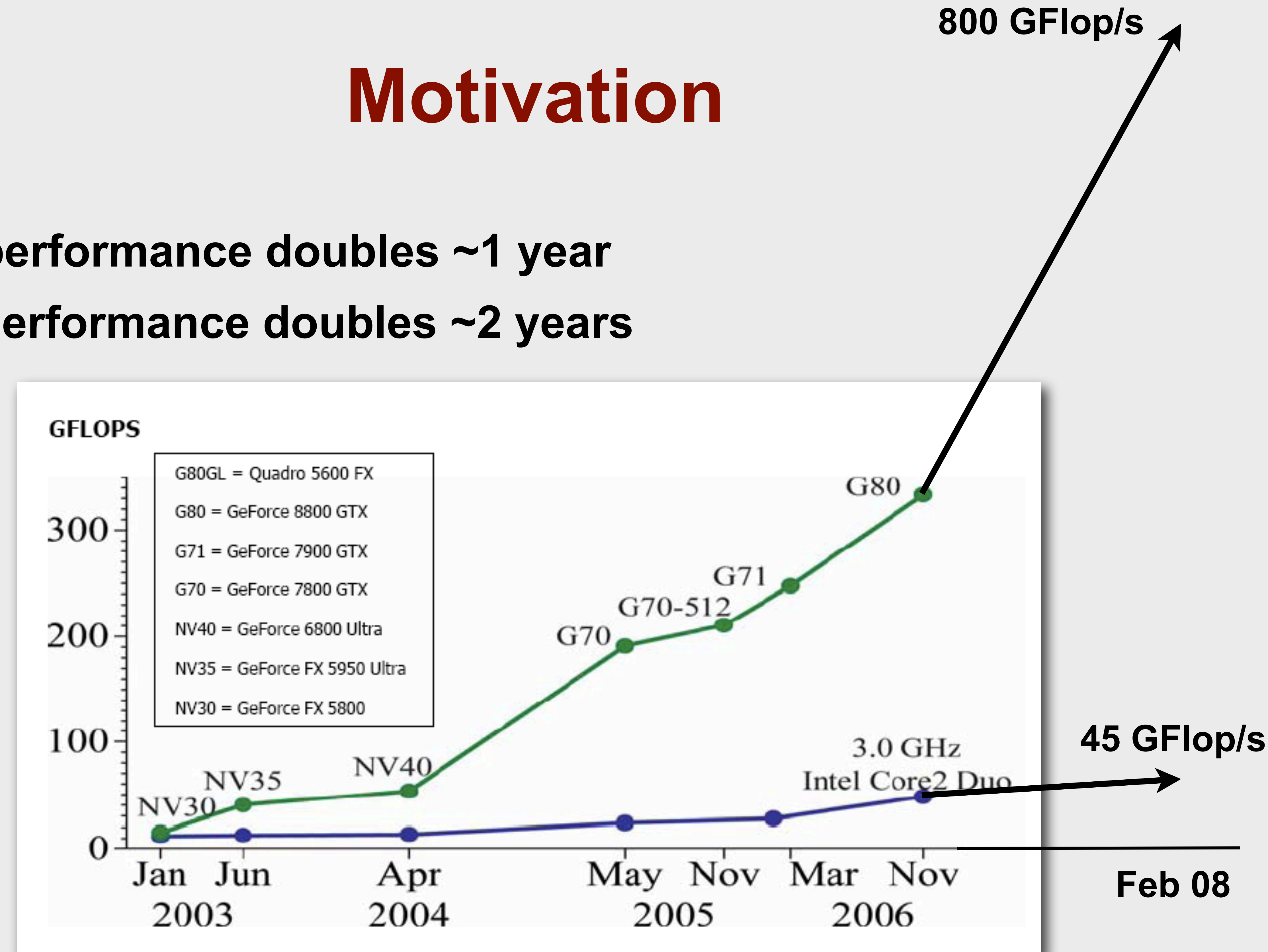

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Lagrangian vortex methods

- **Navier-Stokes equations in vorticity**

$$\frac{D\omega}{Dt} = \omega \cdot \nabla u + \nu \nabla^2 \omega$$

- **Discretized onto Lagrangian particles**

$$\begin{aligned} \bar{\omega}(\bar{x}, t) &= \sum_{i=1}^{N_v} \bar{\Gamma}_i(t)\, \phi_\sigma(\bar{x} - \bar{x}_i) \\ \bar{\Gamma}_i &= \bar{\omega}_i\, \Delta V_i \end{aligned}$$

Why vortex methods?

- *Grid-free* in the fluid domain (only mesh surfaces)
- *Not limited* by CFL convective instability (time steps 10x)
- Computational elements needed only where vorticity present
- *Free* from numerical diffusion (must be explicitly added)
- *Continuity conserved* by construction

CPU-direct method

- **Perform N^2 Biot-Savart evaluations**

$$
\begin{aligned}
\bar{u}_i\left(\bar{x}_i\right) &= \sum_{j=1}^{N_v} K_\sigma\left(\bar{x}_j - \bar{x}_i\right) \times \bar{\Gamma}_j + U_\infty \\
K_\sigma(\bar{x}) &= K(\bar{x}) \int_0^{|\bar{x}|/\sigma} 4\pi\, g(r)\, r^2 dr \\
K(\bar{x}) &= -\frac{\bar{x}}{4\pi|\bar{x}^3|} \\
g(r) &= (3/4\pi)\exp\left(-r^3\right)
\end{aligned}
$$

- **3-component u and 9-component ∇u is 72 Flops**

CPU-direct method

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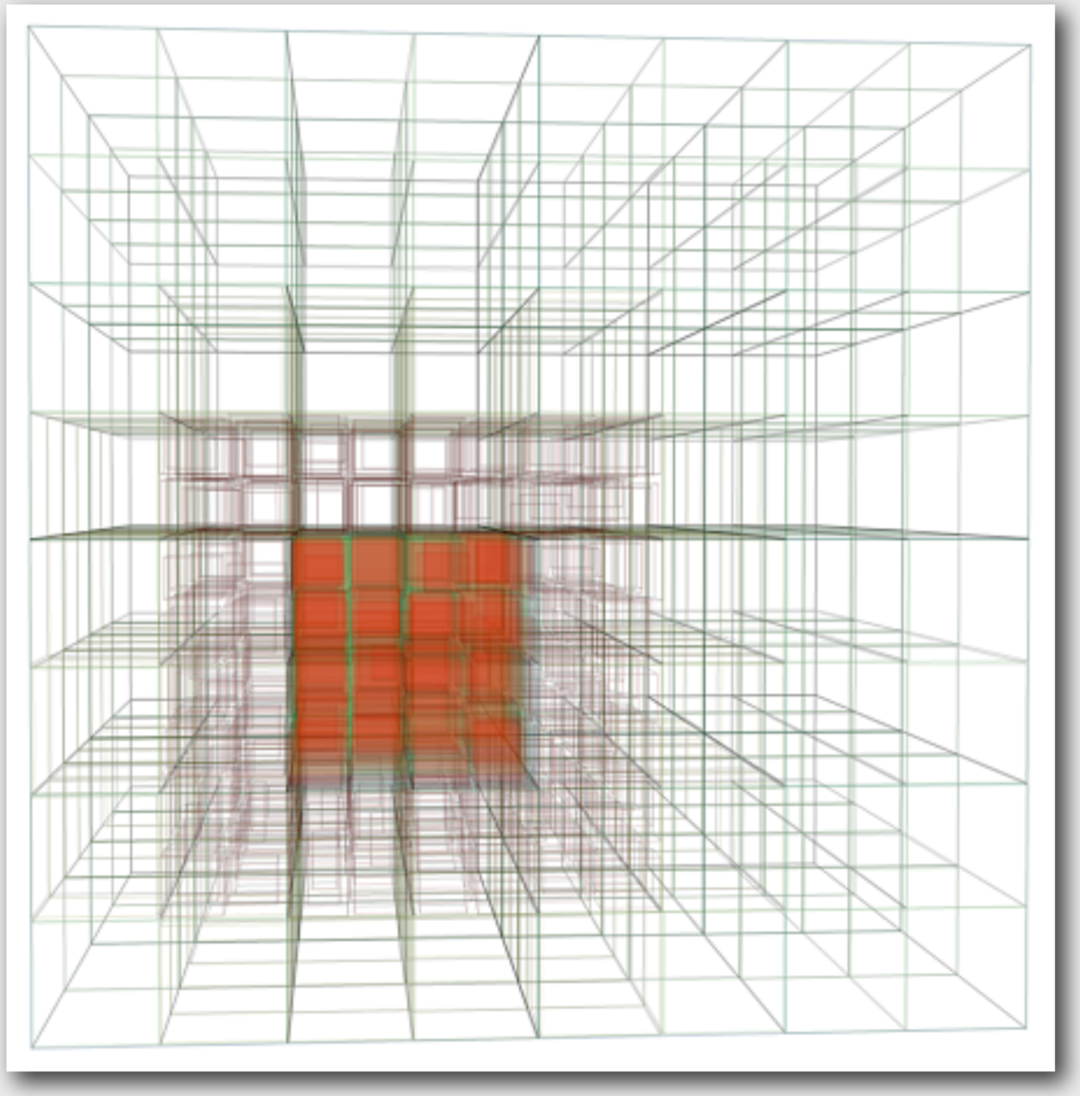
Faster summations

- Appel (1985),
  Barnes and Hut *Treecode* (1986),
  Greengard-Rokhlin *FMM* (1987)
- Principle: use simplified representation for faraway groups of particles
- Application: if box is too close, examine box's children, repeat...
- O(N) to O(N log N)



Our fast multipole treecode

1) **Create tree structure**

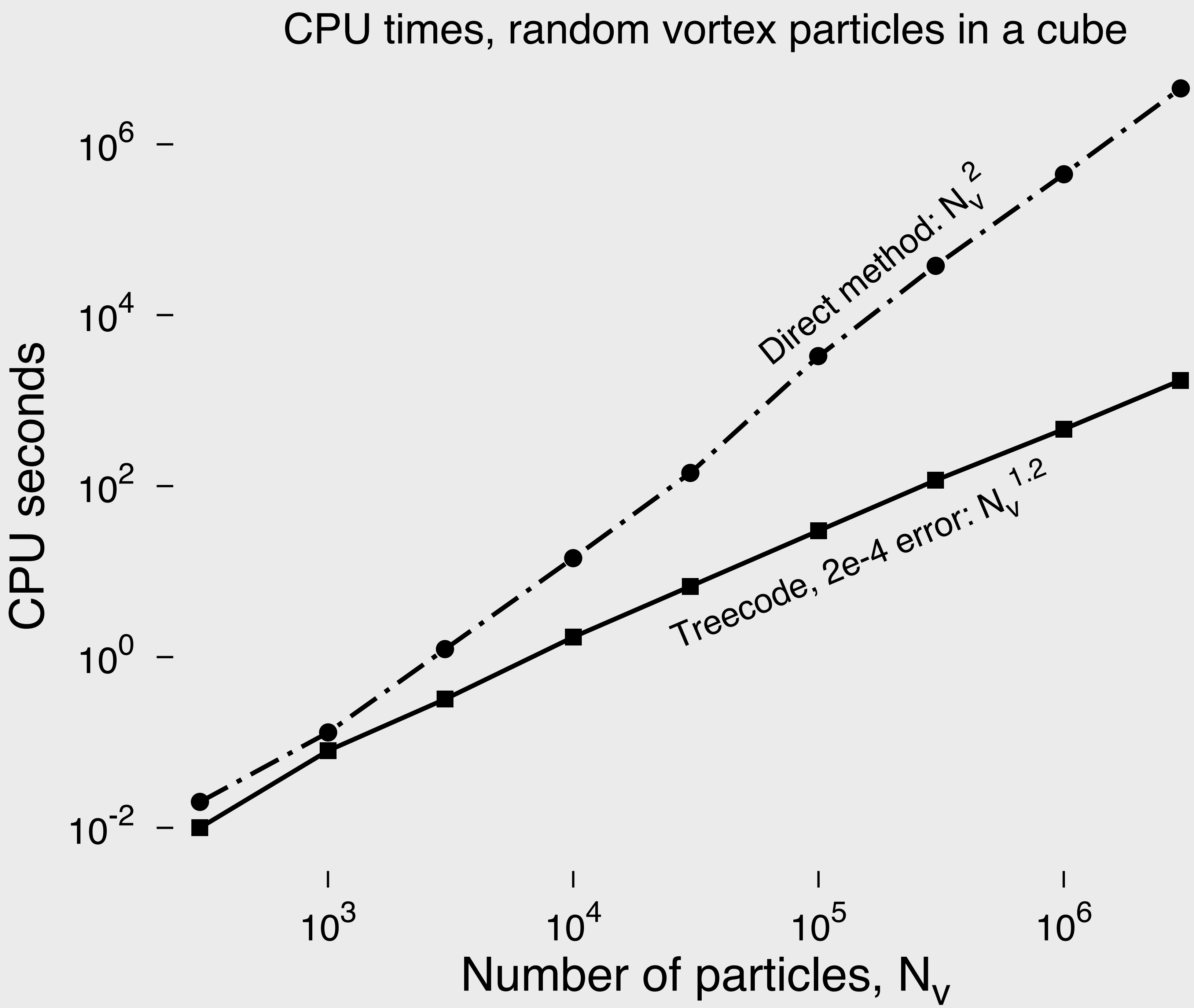
2) **Compute multipole moments for each box**

3) **For each particle:**
   - **Recurse through tree starting at root**
   - **Calculate influence from source box using either multipole multiplication or Biot-Savart, as necessary**
   - **Add freestream**

Our fast multipole treecode

- VAMSplit k-d trees (White and Jain, 1996)
- Only real multipole moments (Wang, 2004)
- 7 or 9 orders of multipole moments
- Barnes-Hut box-opening criteria, with extensions
  Barnes and Hut (1986), Warren and Salmon (1994)
- Interaction lists made uniquely for each particle

Serial performance



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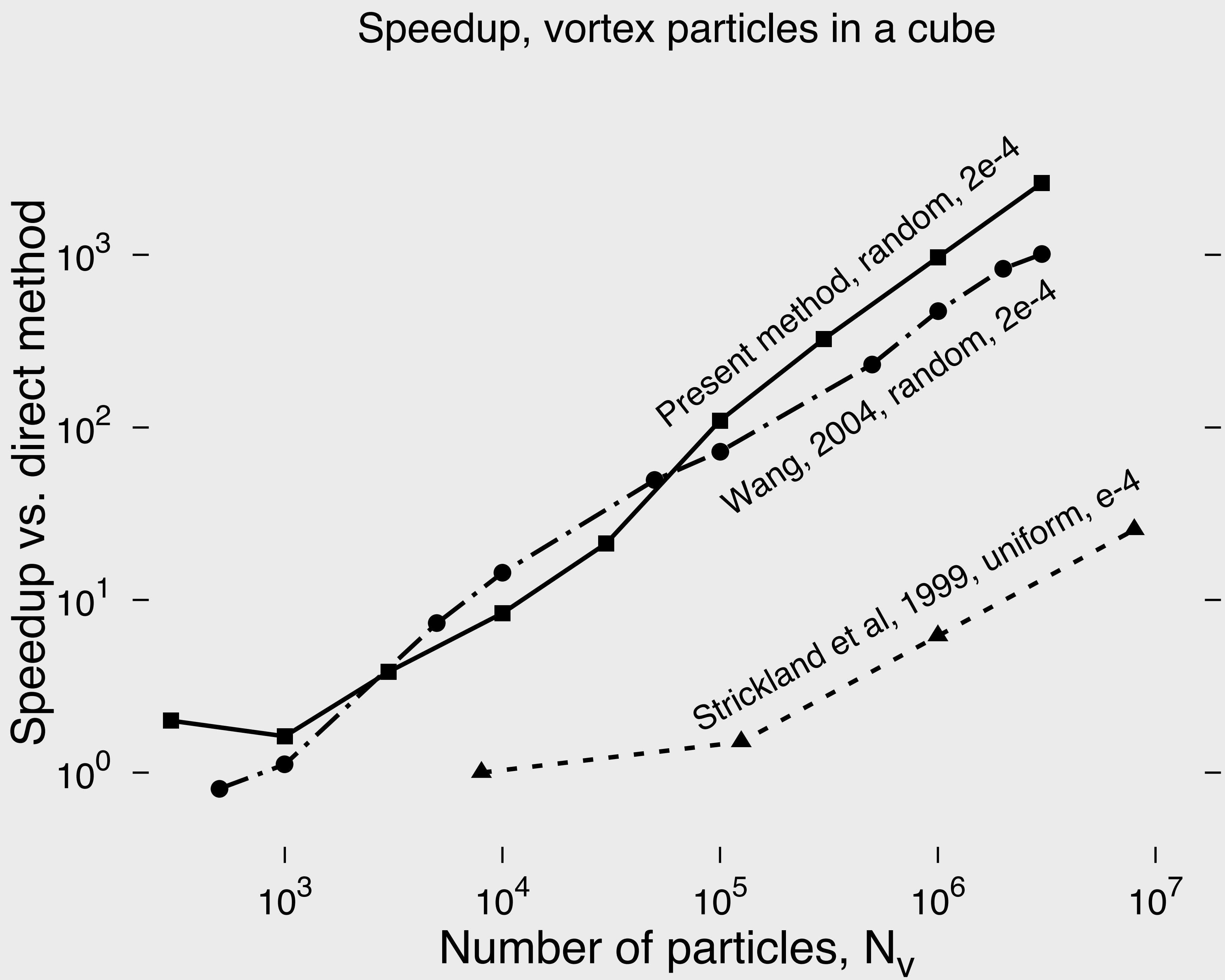
Serial performance



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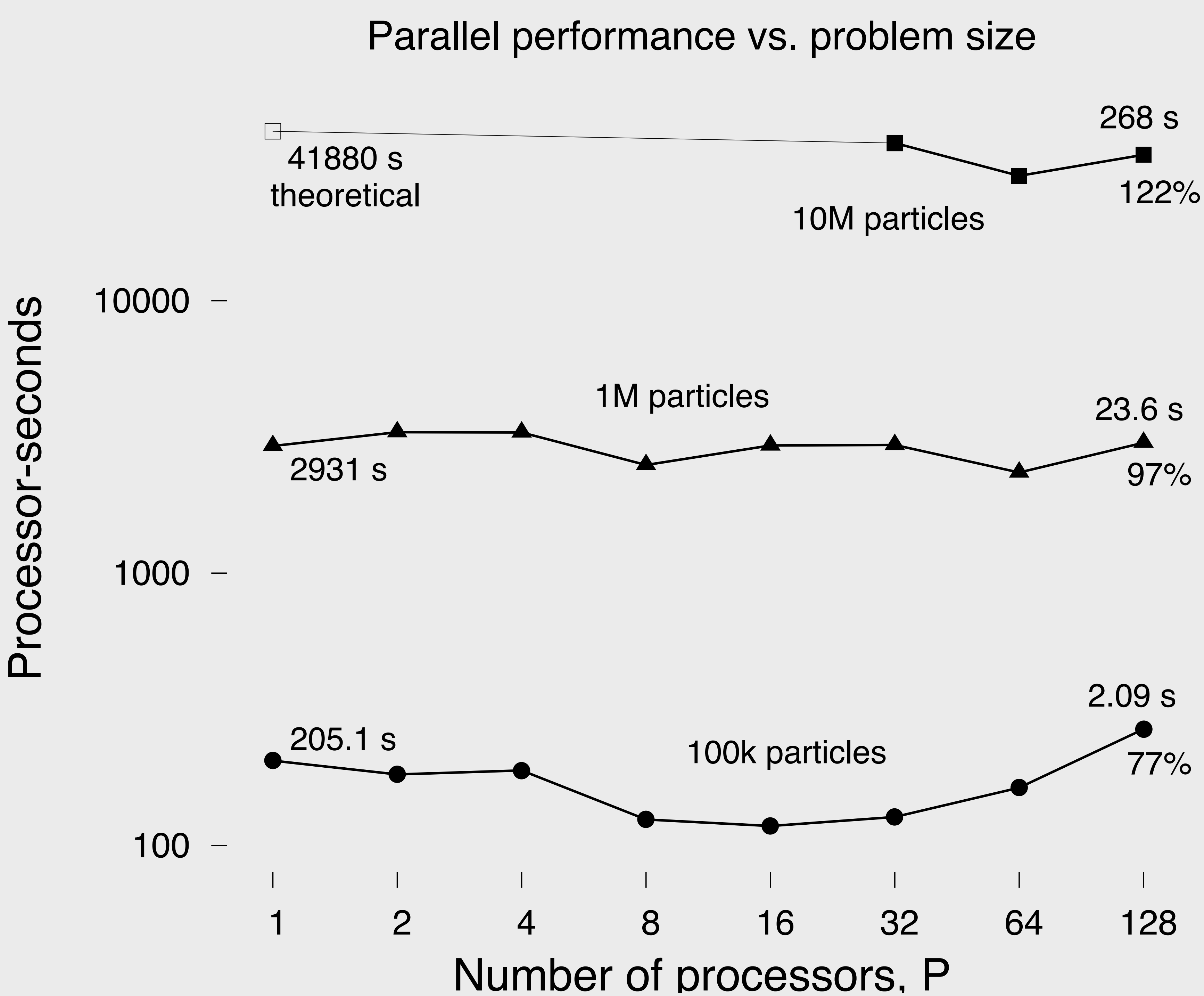
Parallel performance



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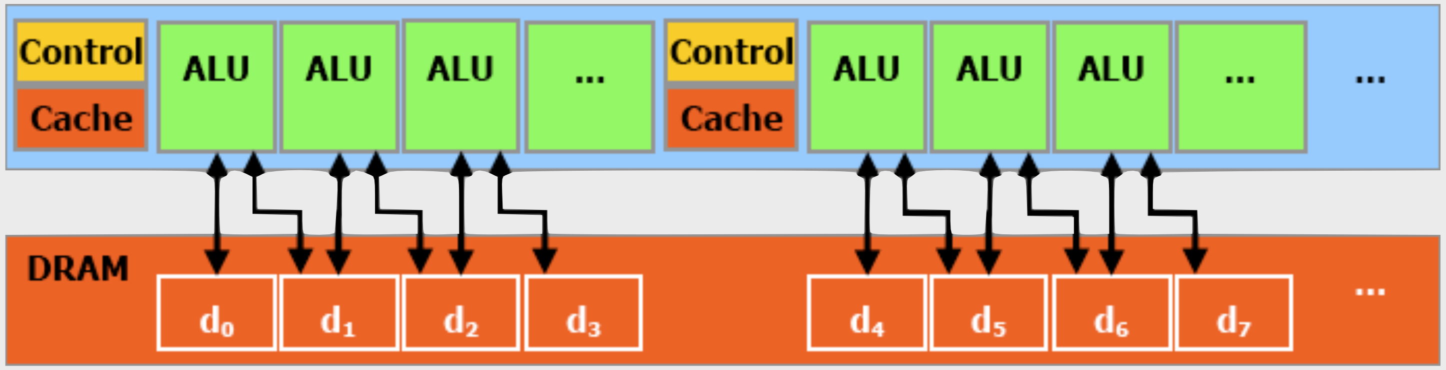
GPU-direct method

- BrookGPU (Buck *et al* 2004)
  - Looks like C language, converted to Cg
  - Define *streams* of data
  - OpenGL driver on Linux returns one set of `float4` per kernel

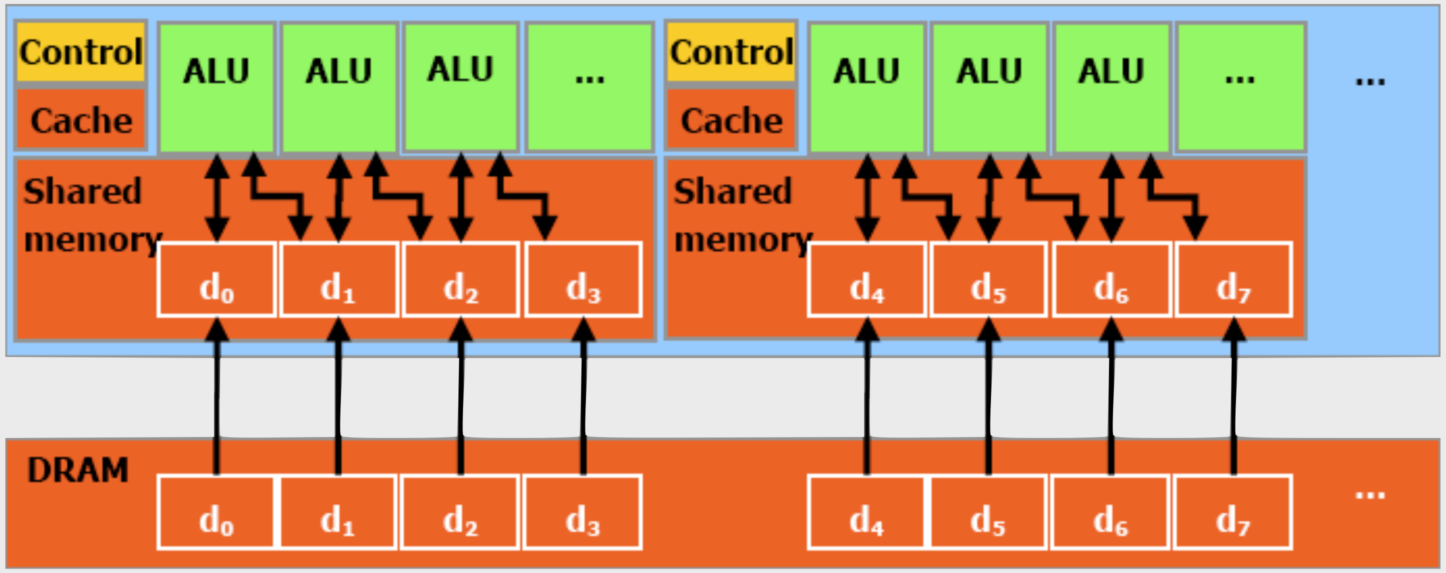
- CUDA: Compute Unified Device Architecture (NVIDIA, 2007)
  - C-like syntax, compiled by nvcc
  - Explicit control of memory on device
  - Kernels have few limits

GPU-direct method

- NVIDIA 8800 GTX has 8 *multiprocessors*, each with:
  - 16 *processing elements* (PEs)
  - 8192 registers
  - 16 banks of 16kB *shared memory*



Without shared memory



With shared memory

GPU-direct method

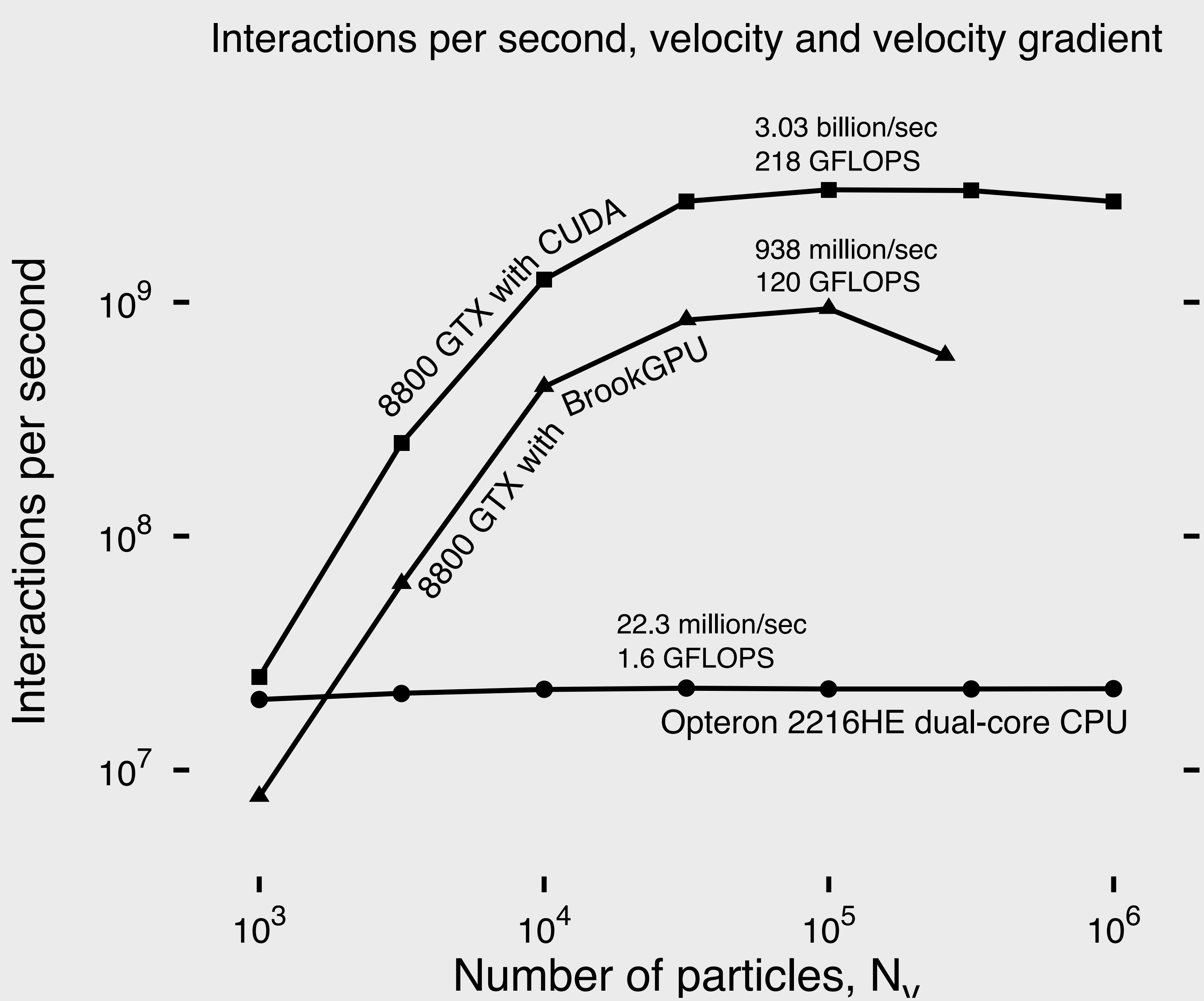
1) Put all particles and field points on GPU main memory

2) Start one thread per field point (8 x 64 = 512 at a time)

3) For each group of 64 threads:
   - Load 64 source particles from main to shared memory
   - Calculate influences using Biot-Savart
   - Repeat; when done, write resulting u and ∇u to main GPU memory

4) Read all u and ∇u back to CPU memory

GPU-direct method



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GPU treecode

1) **Create tree structure (CPU, single-thread)**

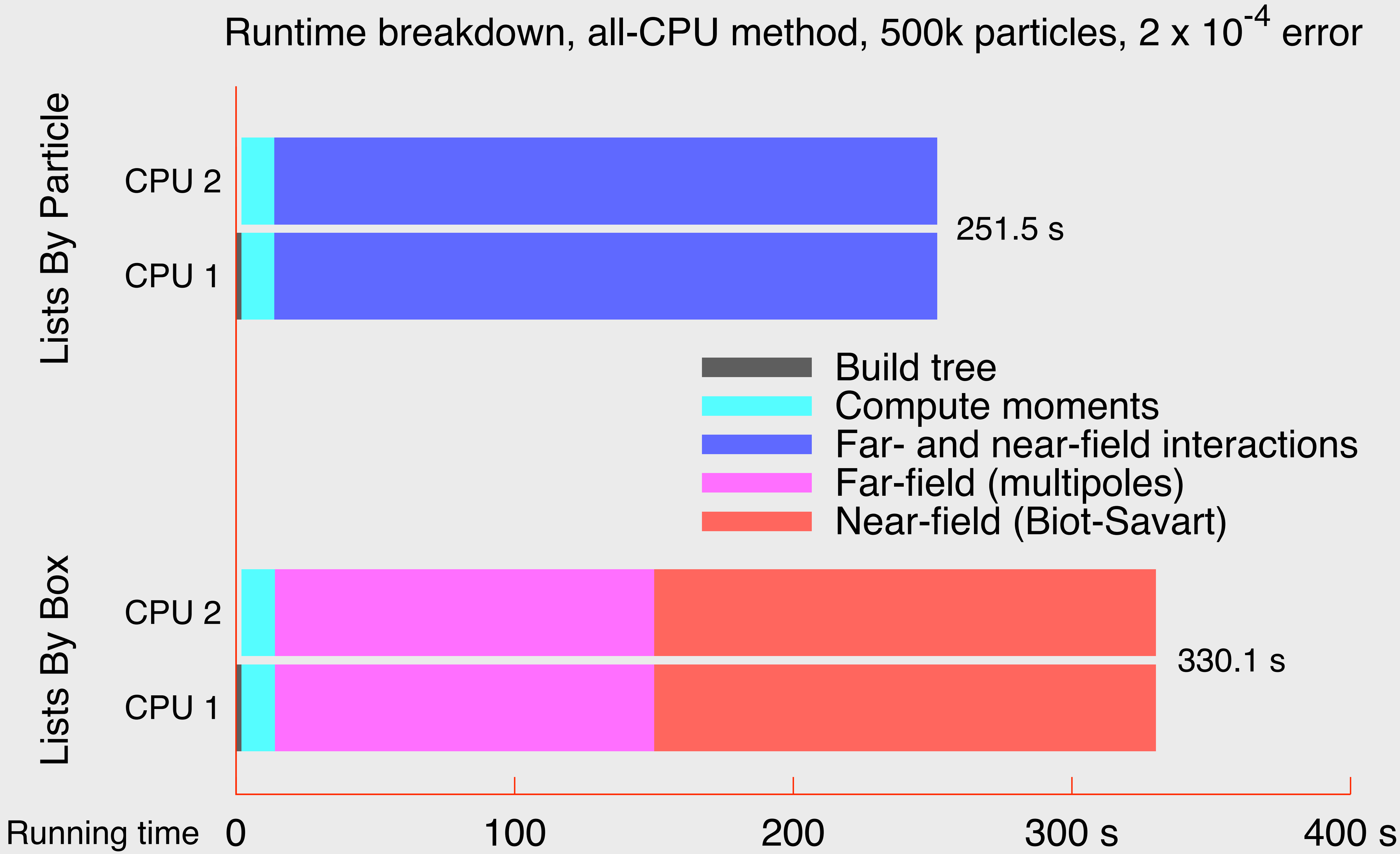
2) **Compute multipole moments for each box (CPU, multithread)**

3) **Determine all interaction lists (CPU, single-thread)**

4) **Calculate all influences from *far-field* using multipole mult. (GPU)**

5) **Calculate all influences from *near-field* using Biot-Savart (GPU)**

GPU treecode



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GPU-direct method -- far-field

1) **Put all particles, field points, and interaction lists on GPU**

2) **Start one thread per field point (8 x 64 = 512 at a time)**

3) **For each group of 64 threads:**
   - **Iterate through that group's *far-field* interaction list**
   - **Load *210 multipole moments* from GPU main to shared memory**
   - **Calculate influences using *multipole multiplication***
   - **Repeat; when done, write resulting u and ∇u to GPU main mem.**

4) **Read all u and ∇u back to CPU main memory**

GPU-direct method -- near-field

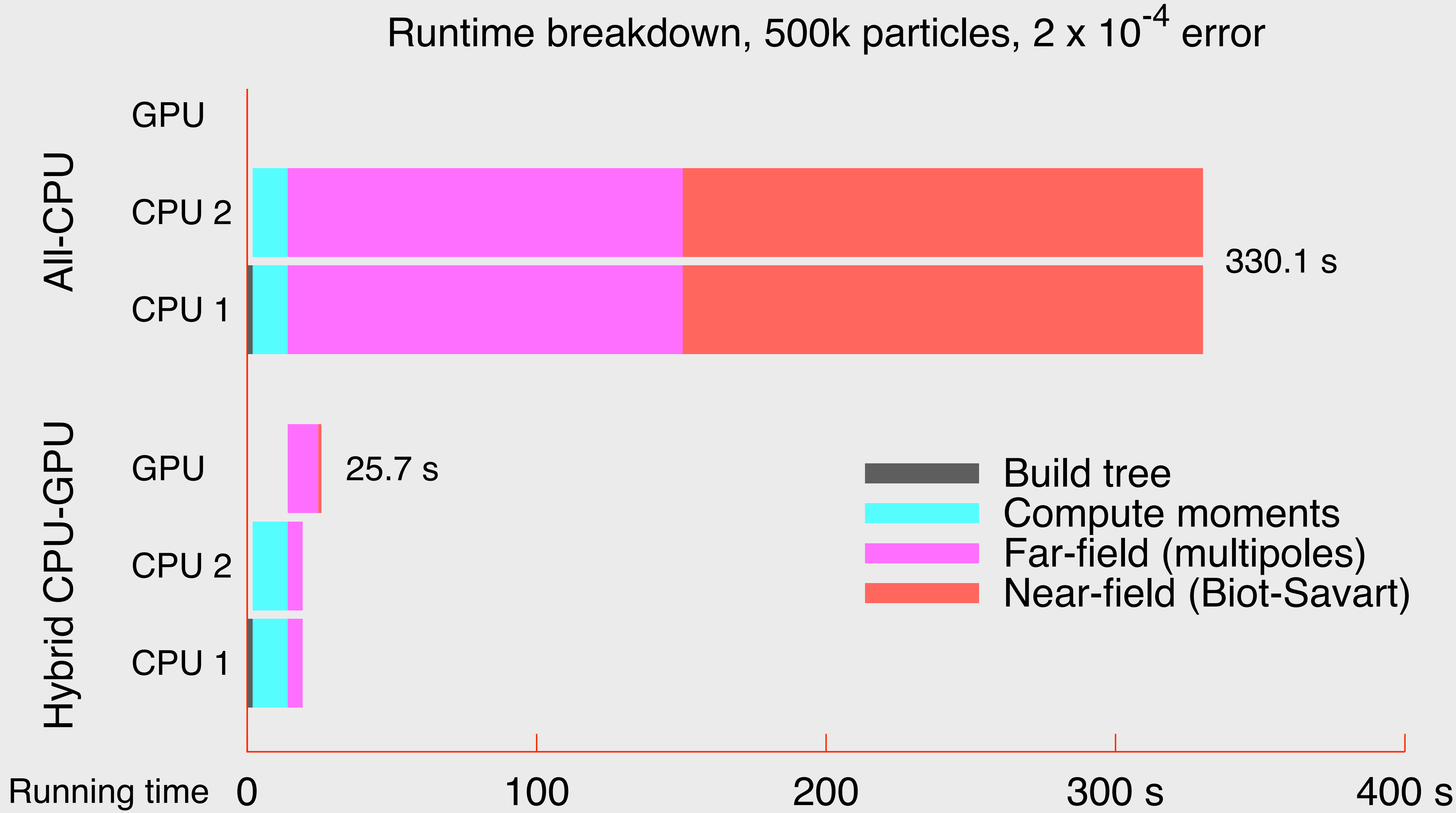
1) **Put all particles, field points, and interaction lists on GPU**

2) **Start one thread per field point (8 x 64 = 512 at a time)**

3) **For each group of 64 threads:**
   - **Iterate through that group's *near-field* interaction list**
   - **Load *64 source particles* from GPU main to shared memory**
   - **Calculate influences using *Biot-Savart***
   - **Repeat; when done, write resulting u and ∇u to GPU main mem.**

4) **Read all u and ∇u back to CPU main memory**

GPU treecode



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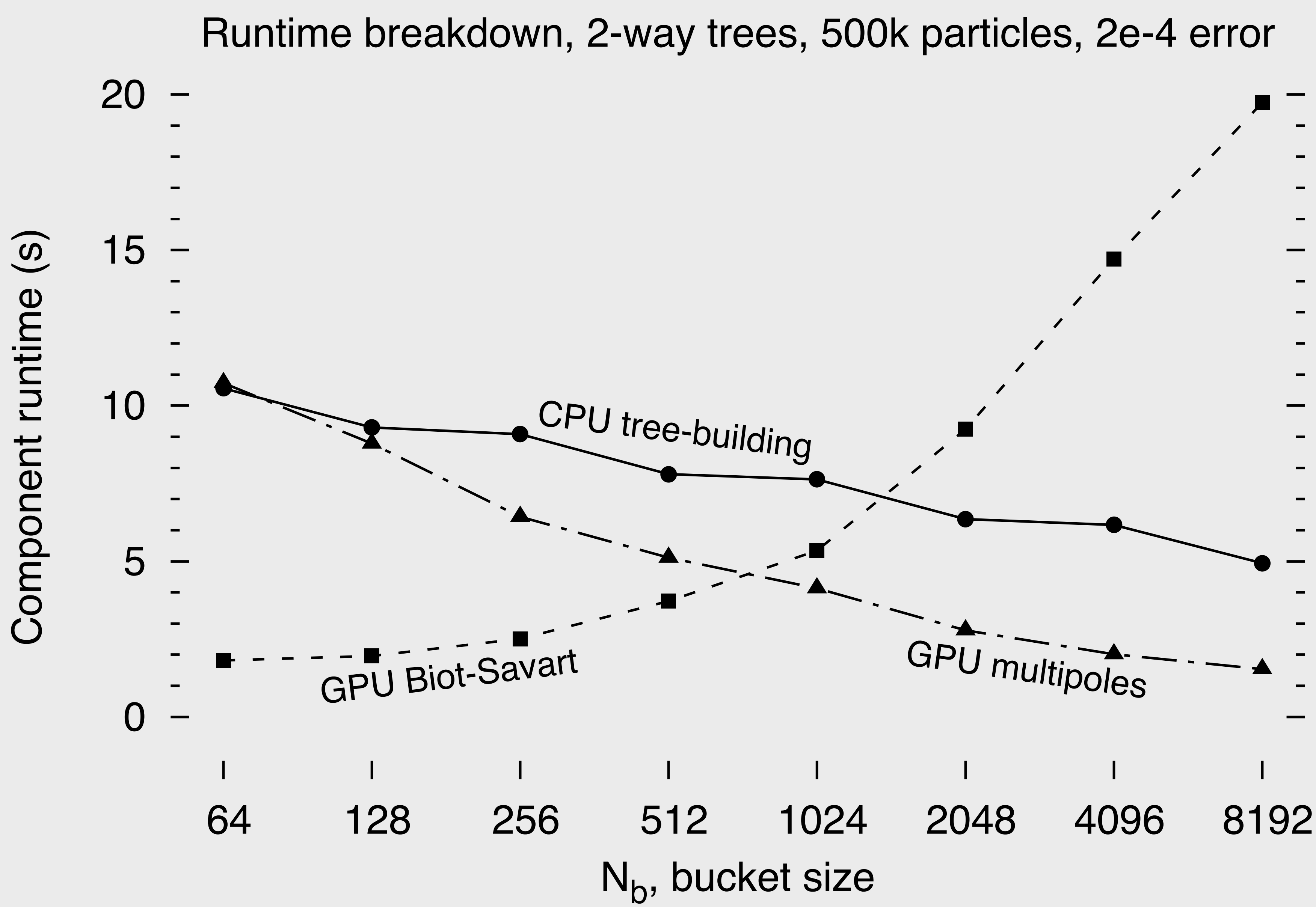
GPU treecode

- Changing *bucket size* shifts work between near- and far-field



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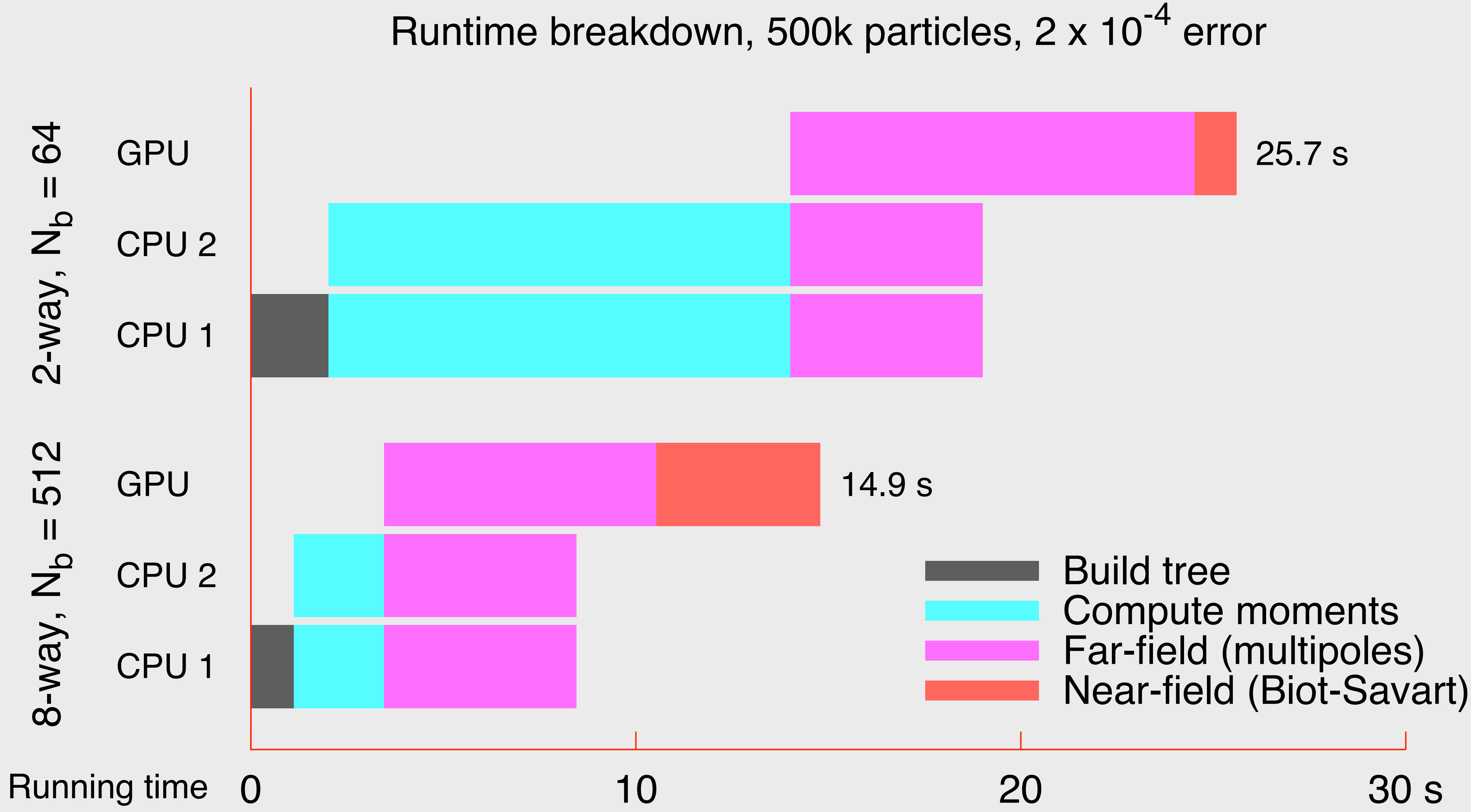
GPU treecode



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Best performance, 500k particles, 2×10^{-4} mean velocity error

	Total time	Tree-building	Multipole moments	Velocity solution
CPU direct	11242 s	-	-	11242 s
CPU treecode	251.5 s	2.0 s	11.7 s	237.8 s
GPU direct	88.7 s	-	-	88.7 s
GPU treecode	14.9 s	1.1 s	2.3 s	11.4 s

Dynamic simulation step

- **Inviscid Flow - Lagrangian Vortex Element Method**

$$\frac{\partial \bar{x}_i}{\partial t} = \bar{u}_i$$

$$\frac{\partial \bar{\Gamma}_i}{\partial t} = \bar{\Gamma}_i \cdot \nabla \bar{u}_i$$

- **Diffusion - Vorticity Redistribution** (Shankar and van Dommelen, 1996)

$$\frac{\partial \bar{\Gamma}_i}{\partial t} = \nu \nabla^2 \bar{\Gamma}_i$$

Dynamic simulation step

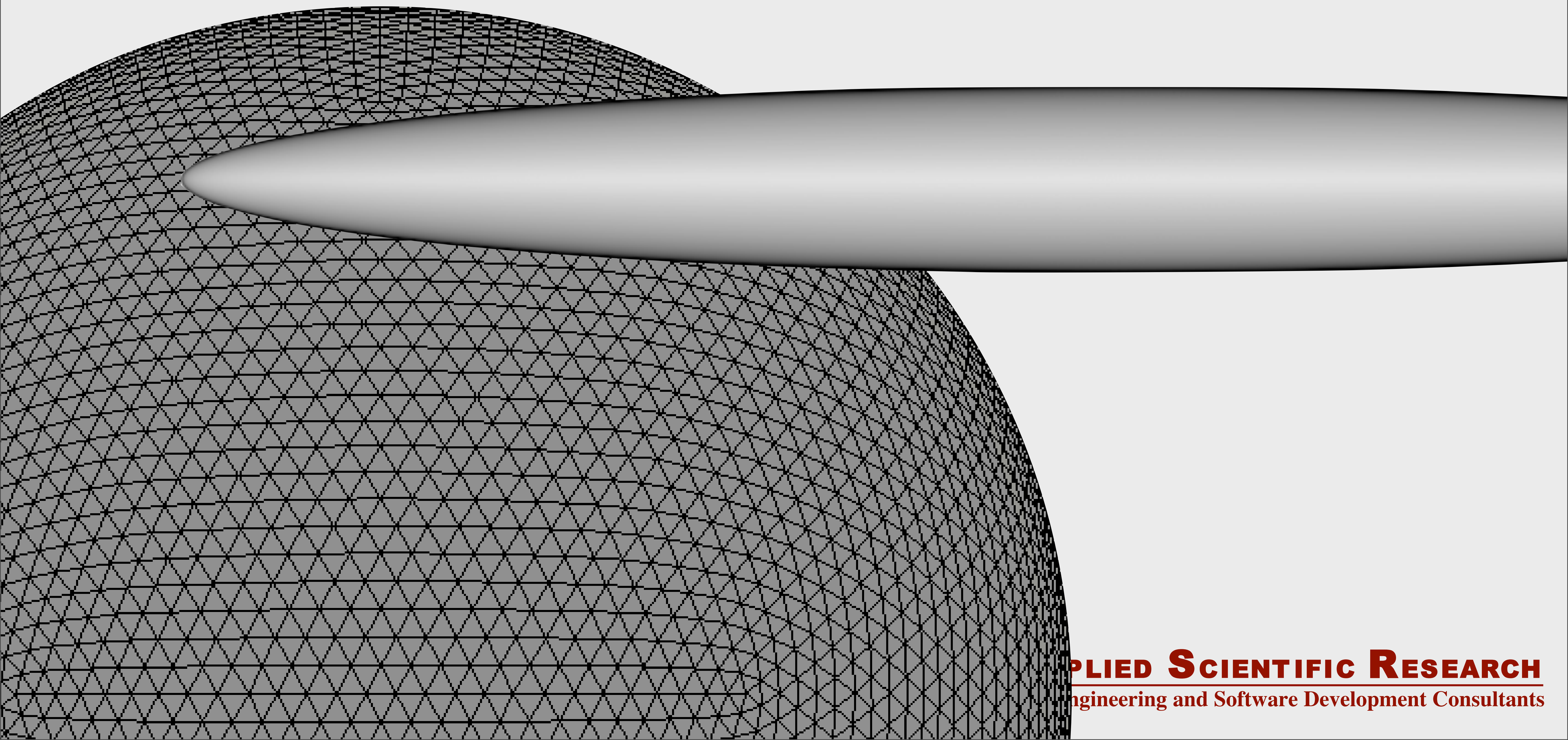
- **Wall B.C. satisfied by generating vorticity at the wall -**
  Boundary Element Method

$$\frac{1}{2}(\bar{\gamma}A)_i \times \hat{n} + \sum_{m \neq i}^{N_v} (\bar{\gamma}A)_m \times \int_{S_i} K(\bar{x} - \bar{x}_m)\, d\bar{x} = \bar{Q}_s$$

$$\bar{Q}_s = \int_{S_i} \bar{U}_\infty(\bar{x})\, d\bar{x} - \sum_{j=1}^{N_v} \bar{\Gamma}_j \times \int_{S_i} K(\bar{x} - \bar{x}_j)\, d\bar{x}$$

Flow over 10:10:1 ellipsoid at 60°
Re_D=1000

SURFACE MESH



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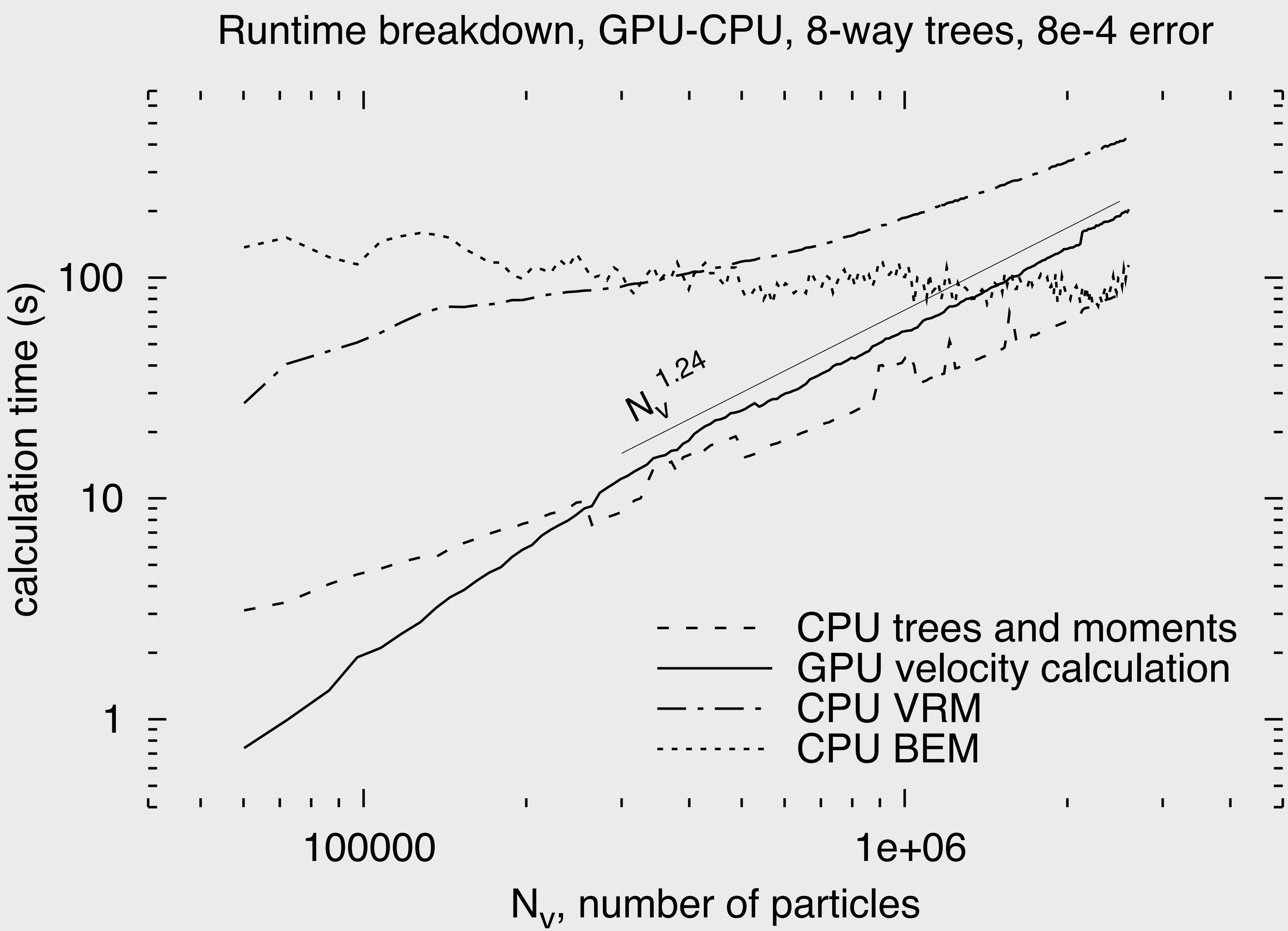

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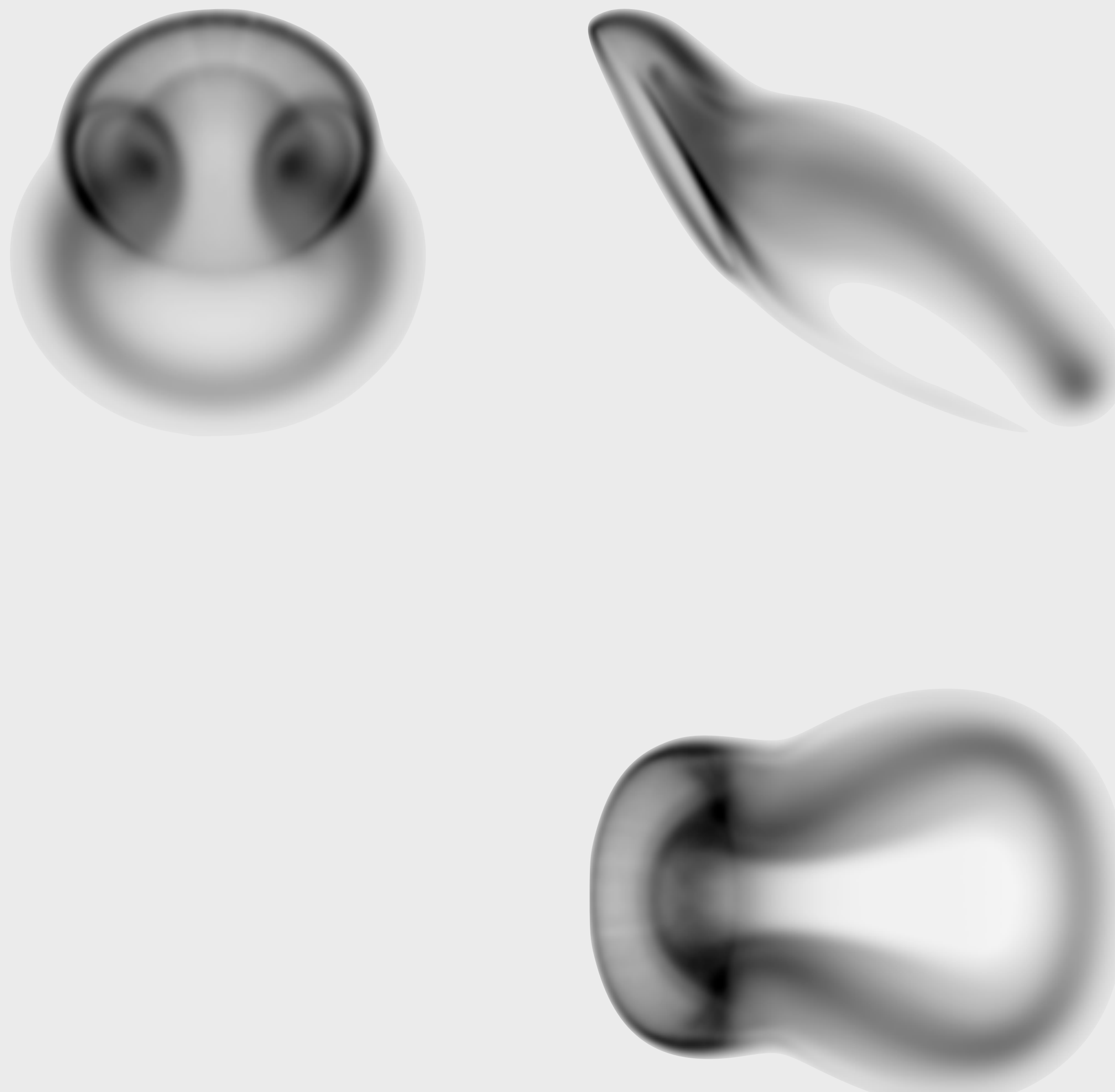

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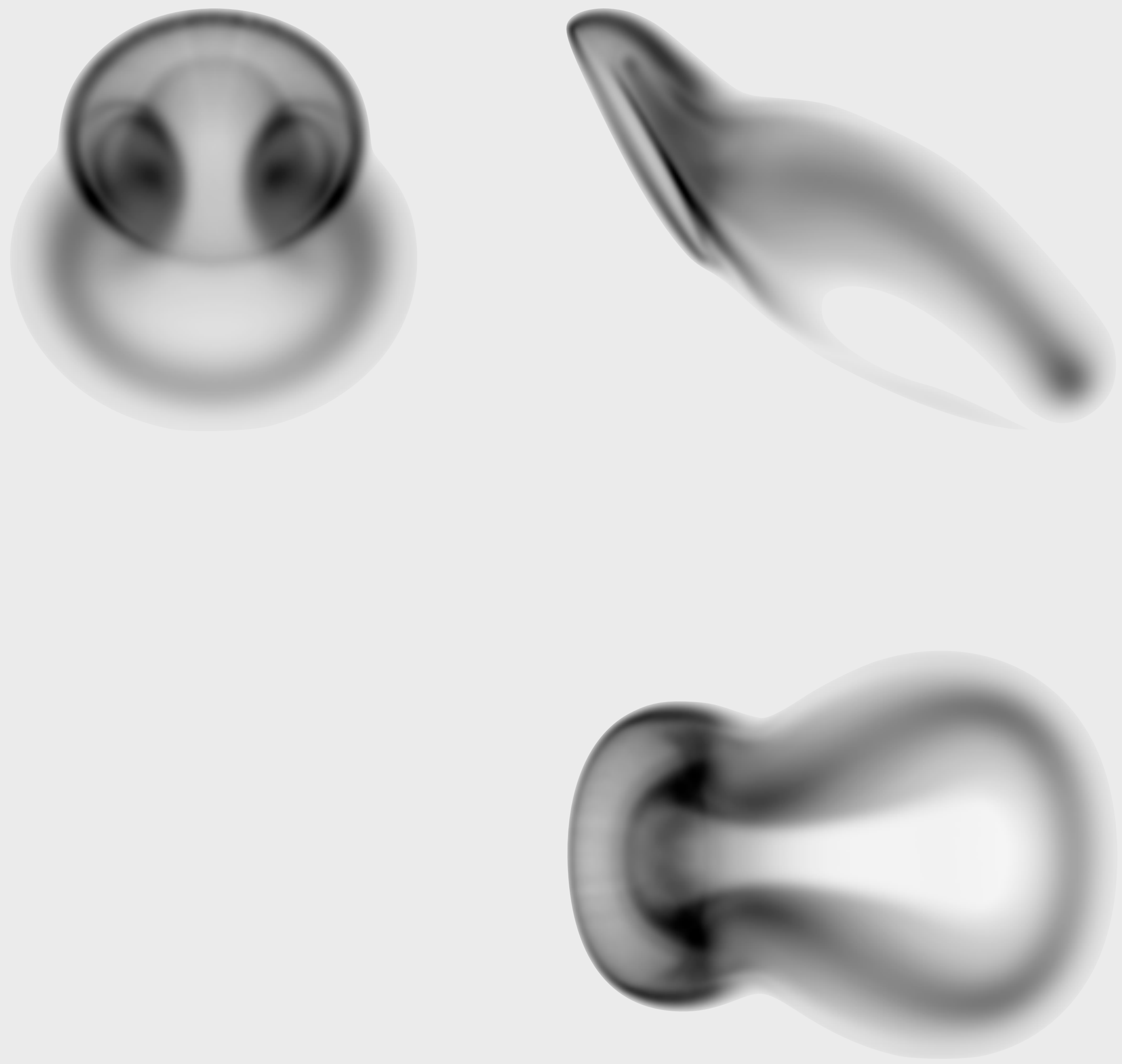

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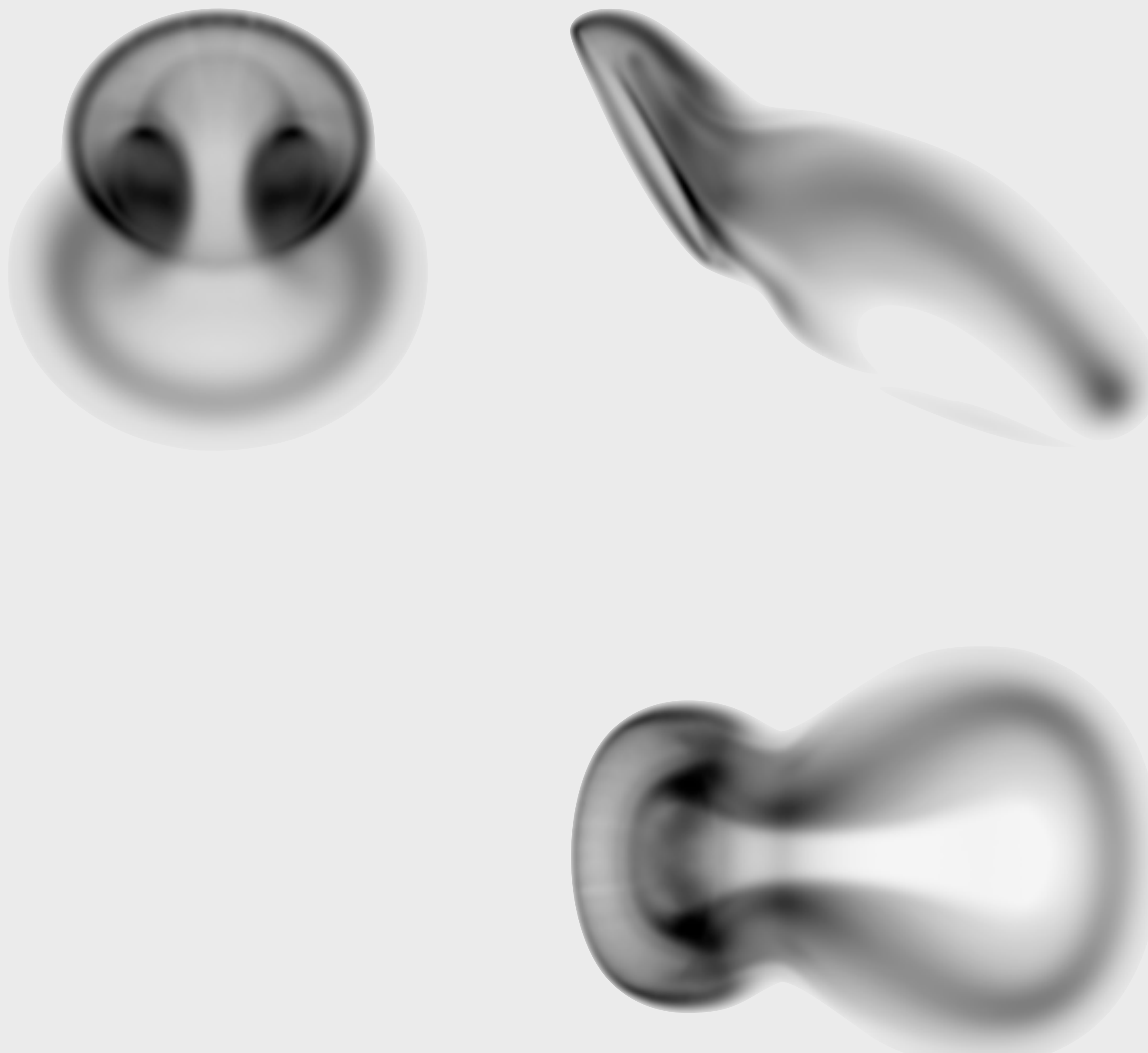

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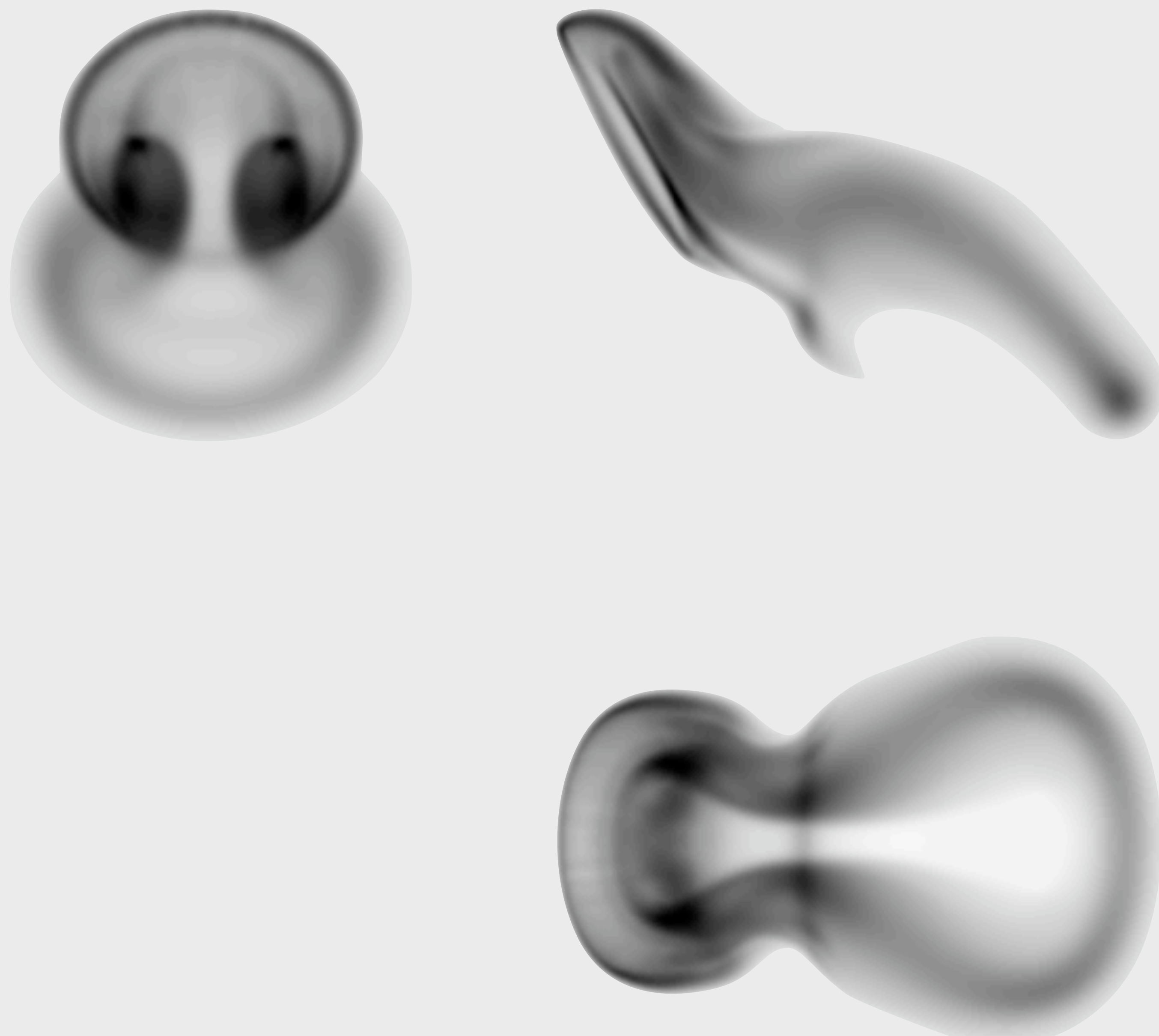

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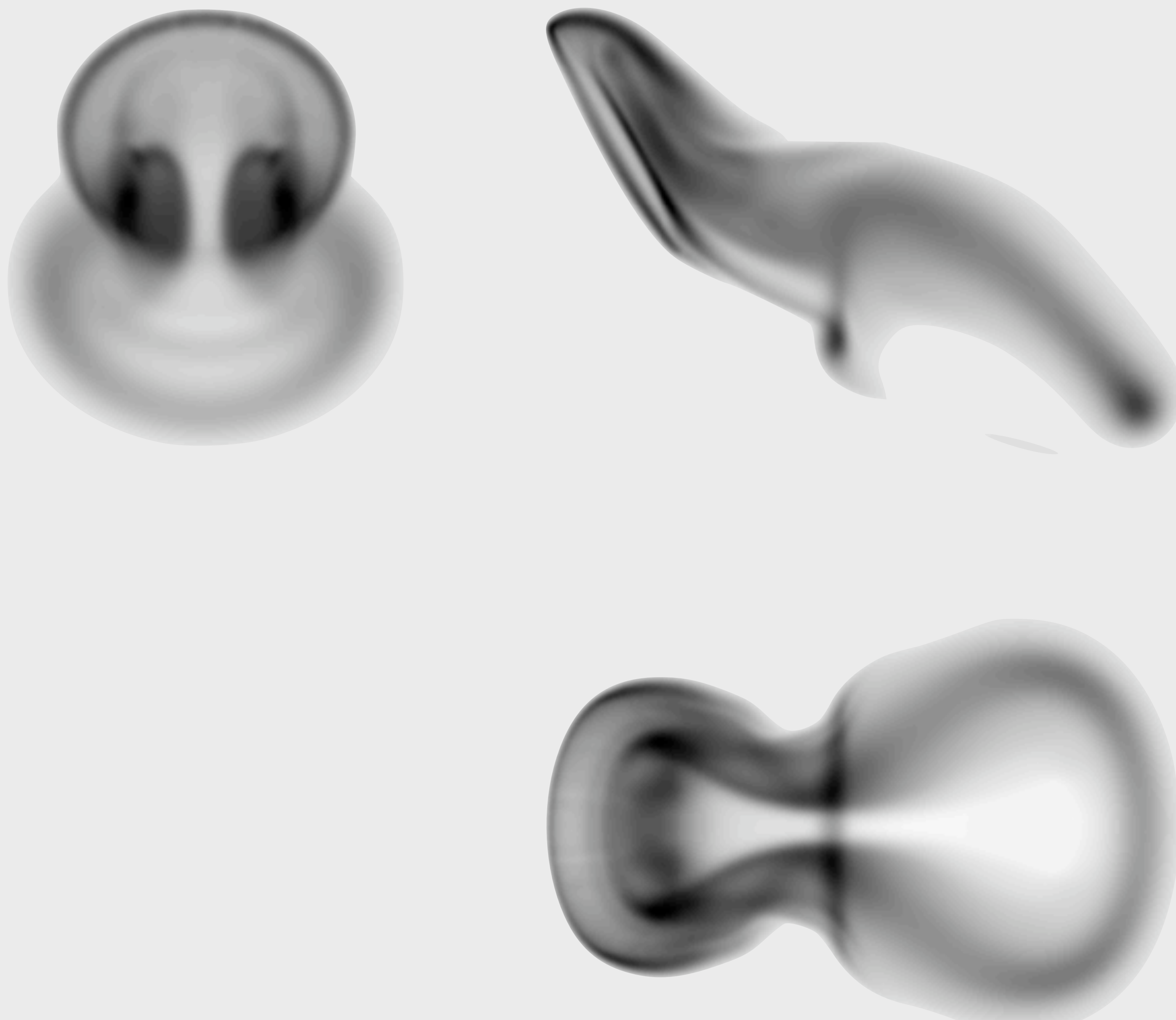

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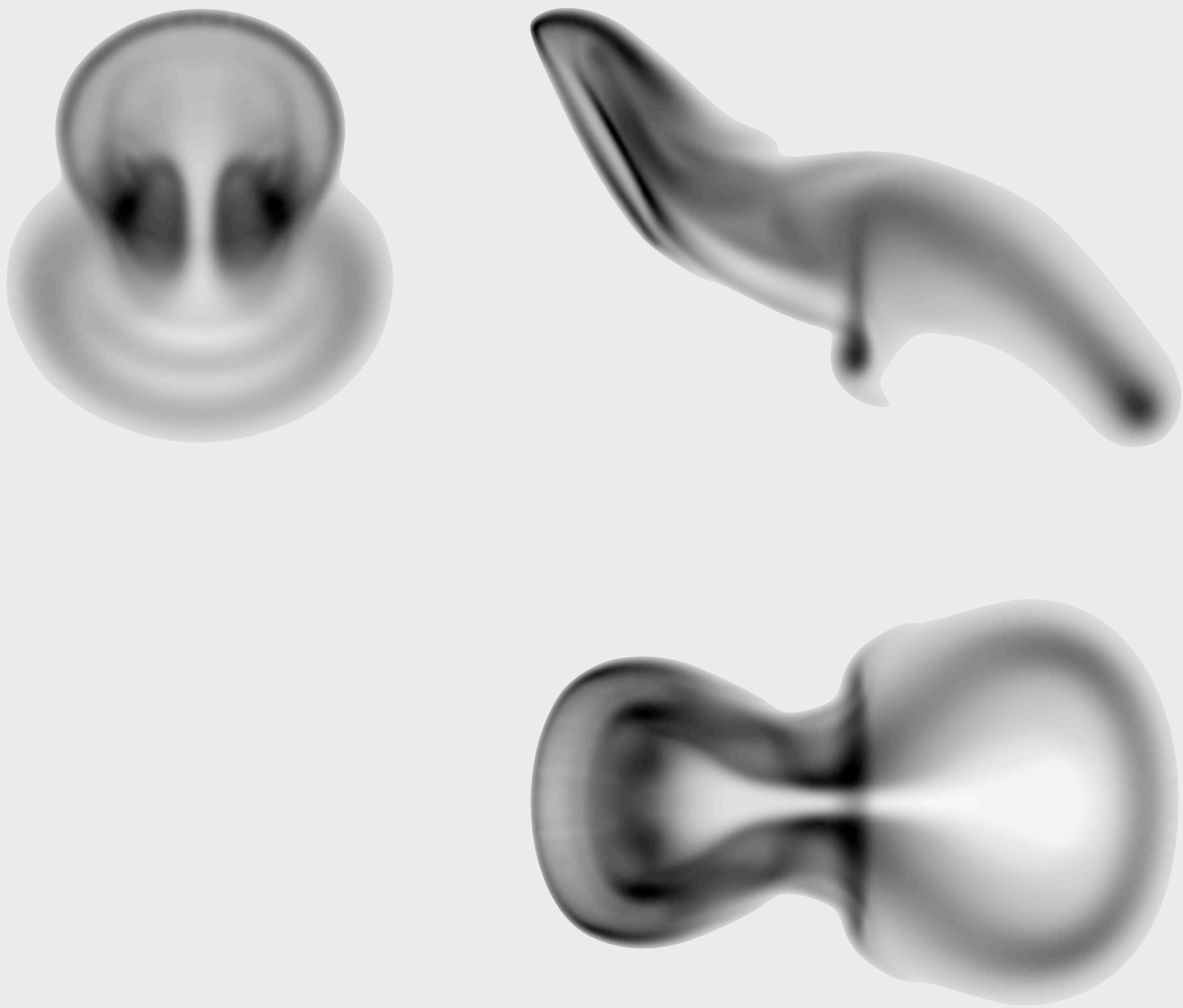

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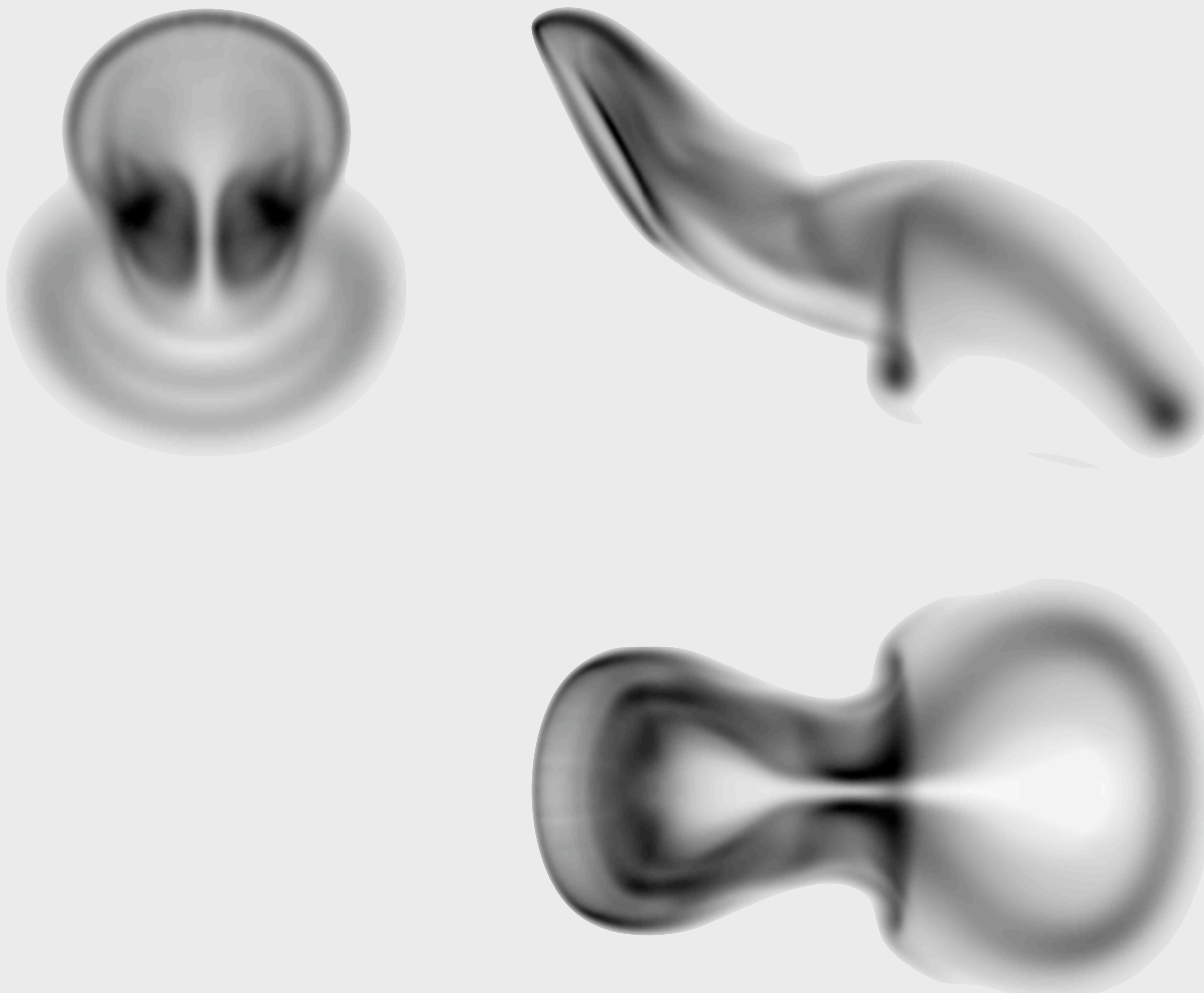

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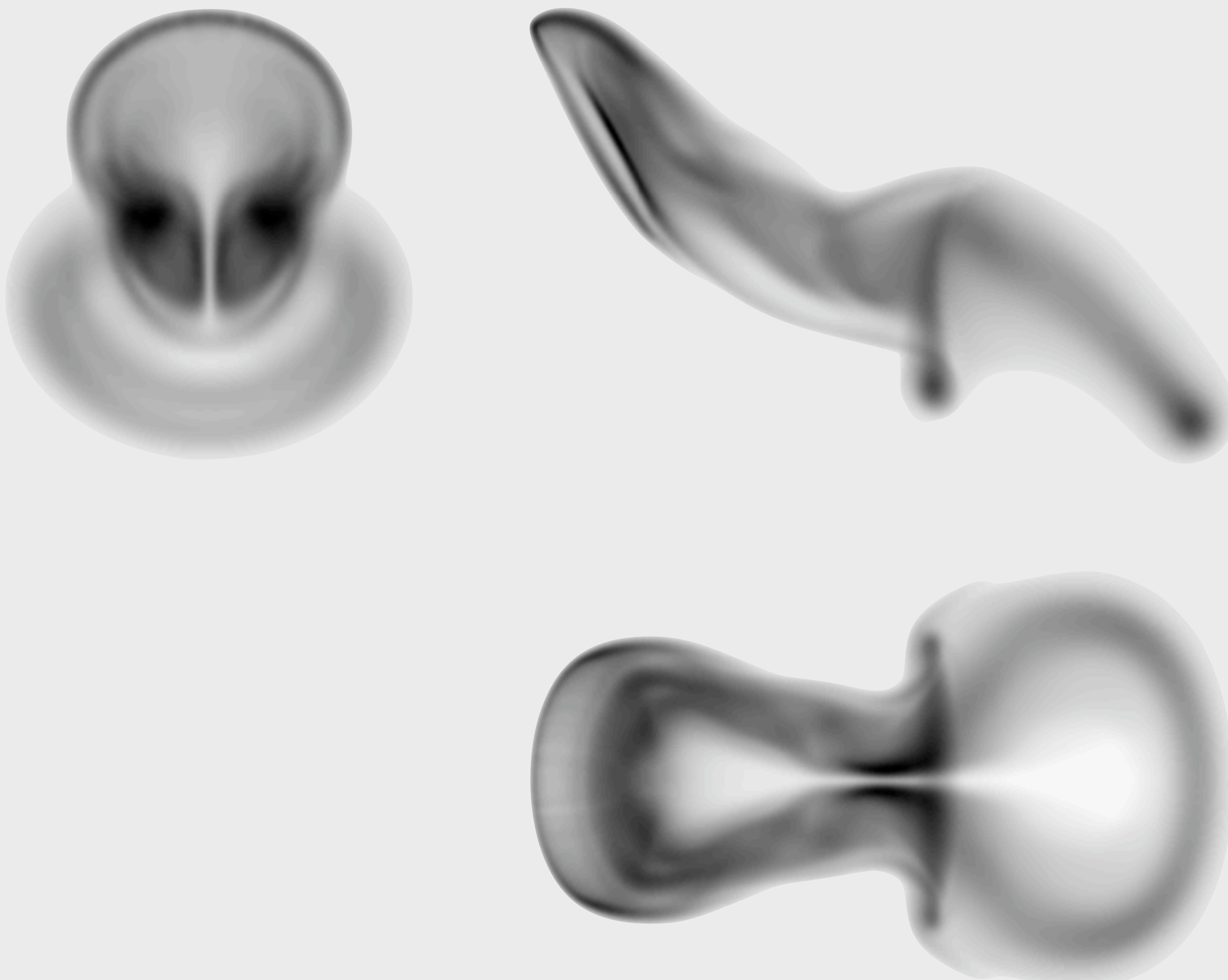

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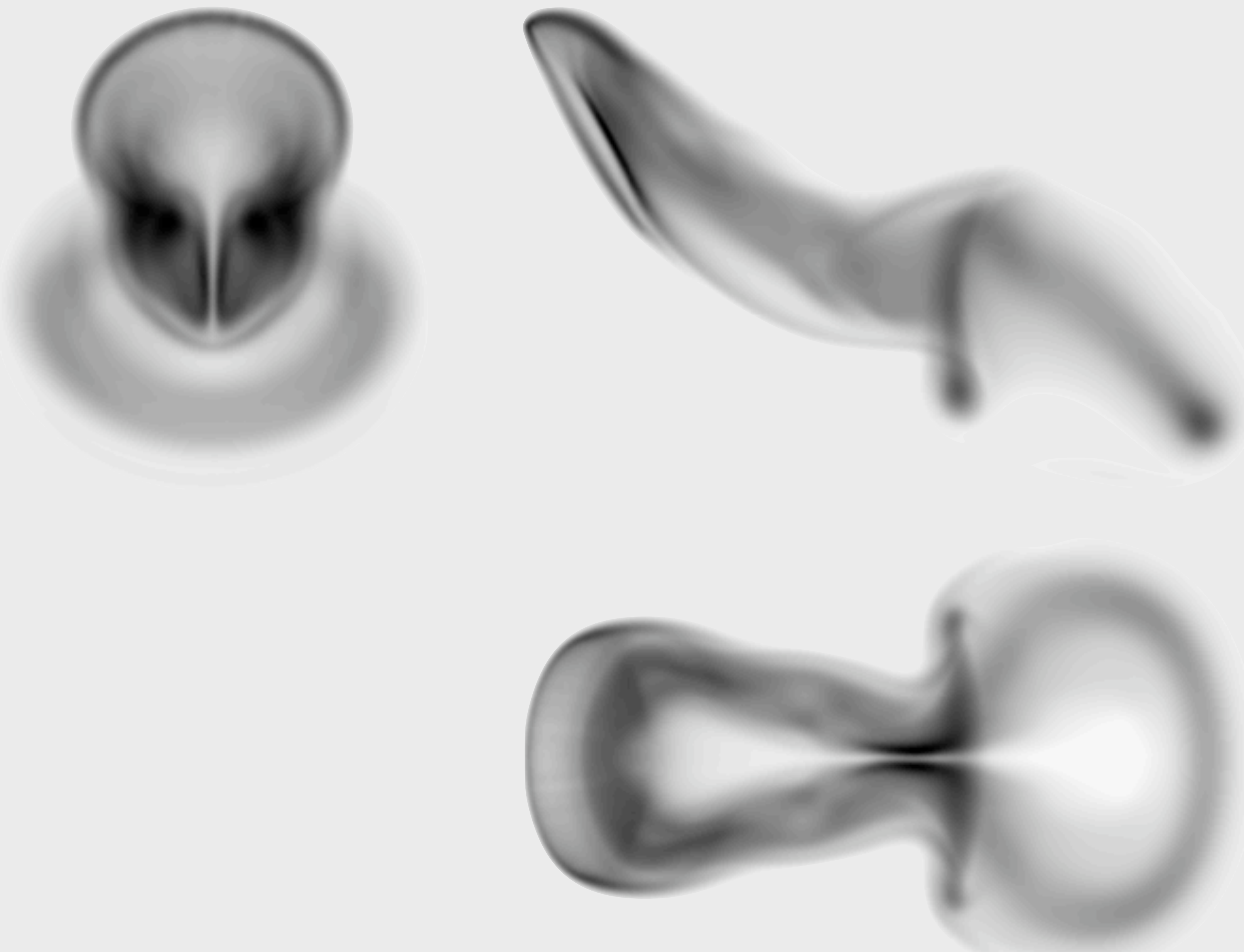

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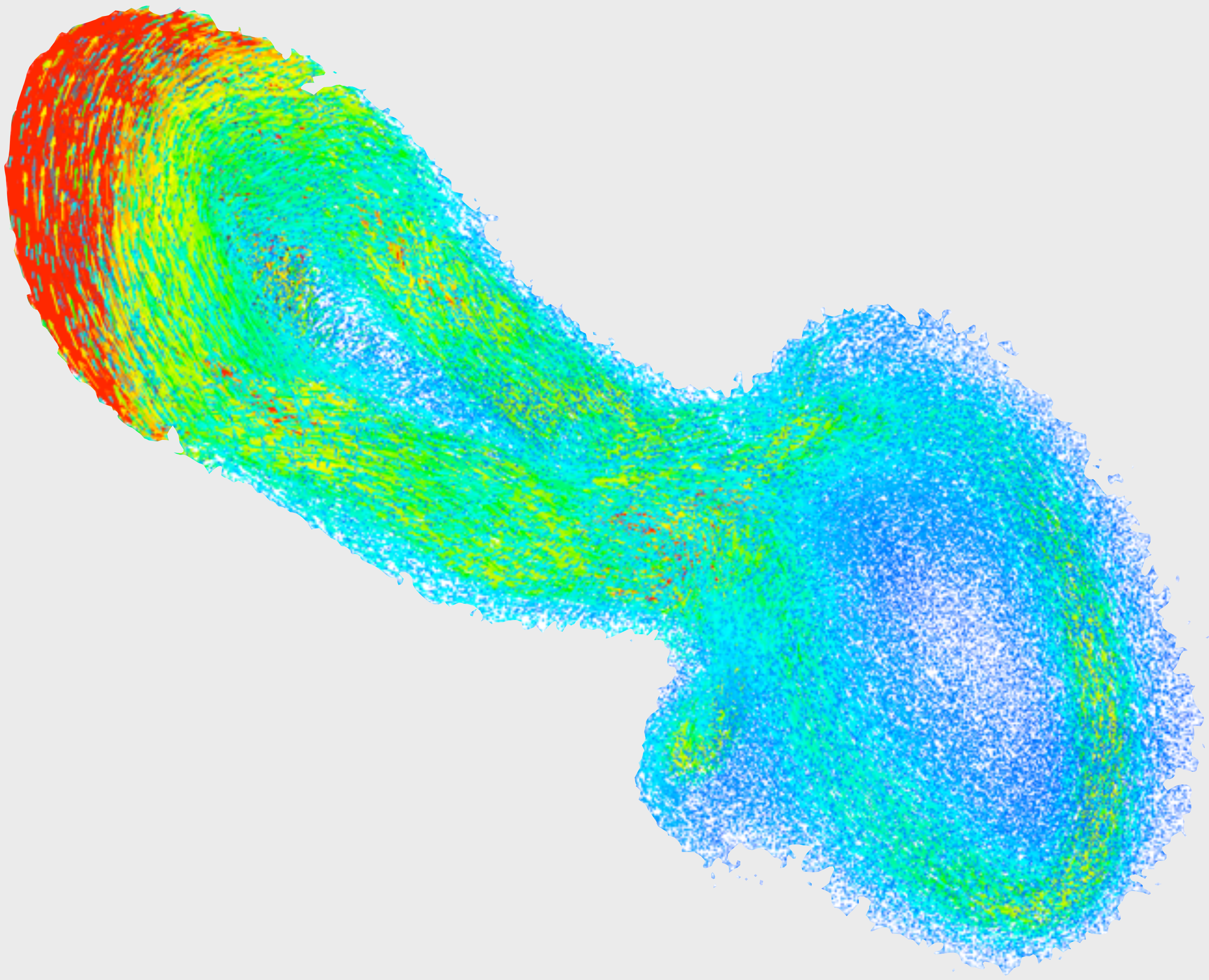

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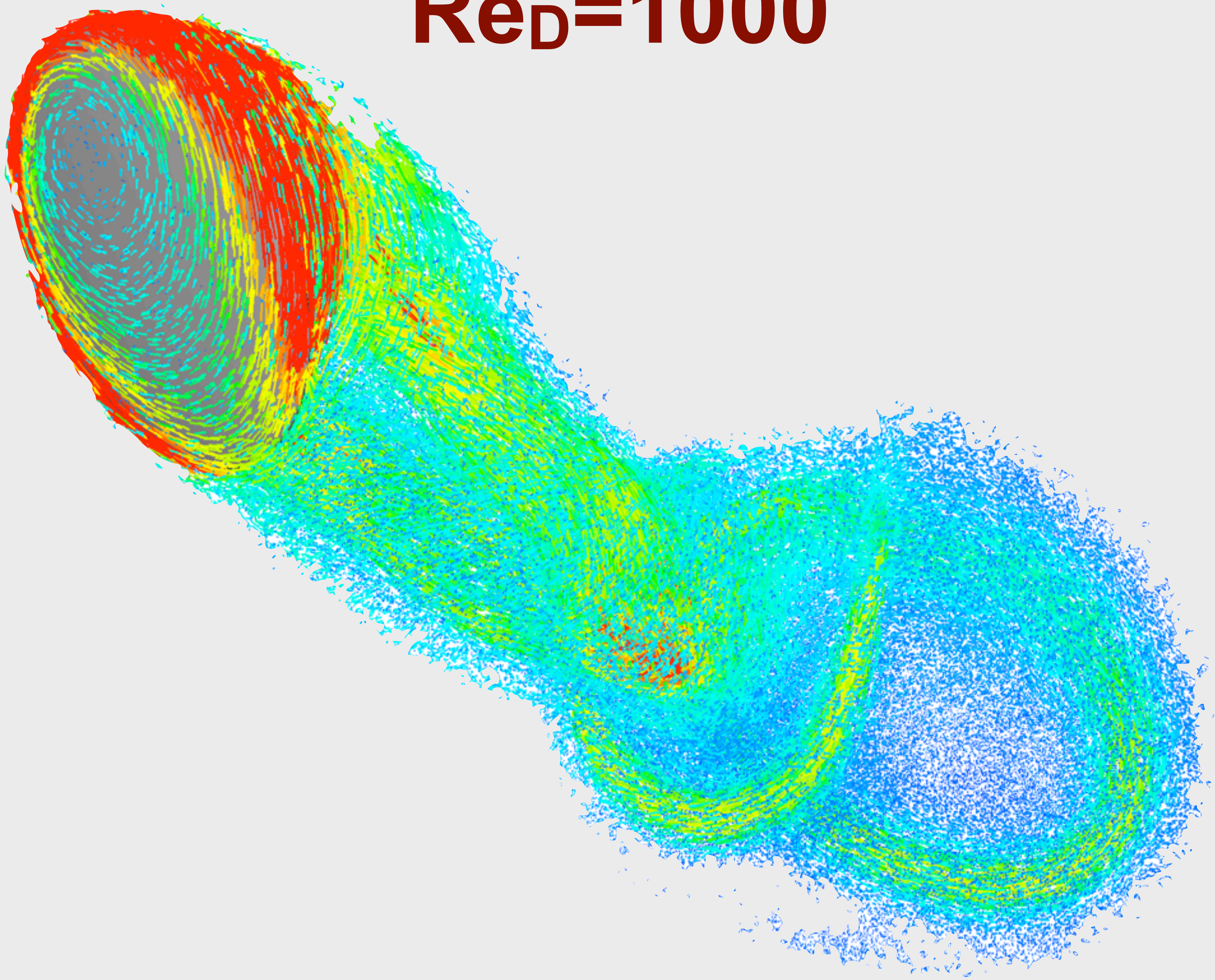

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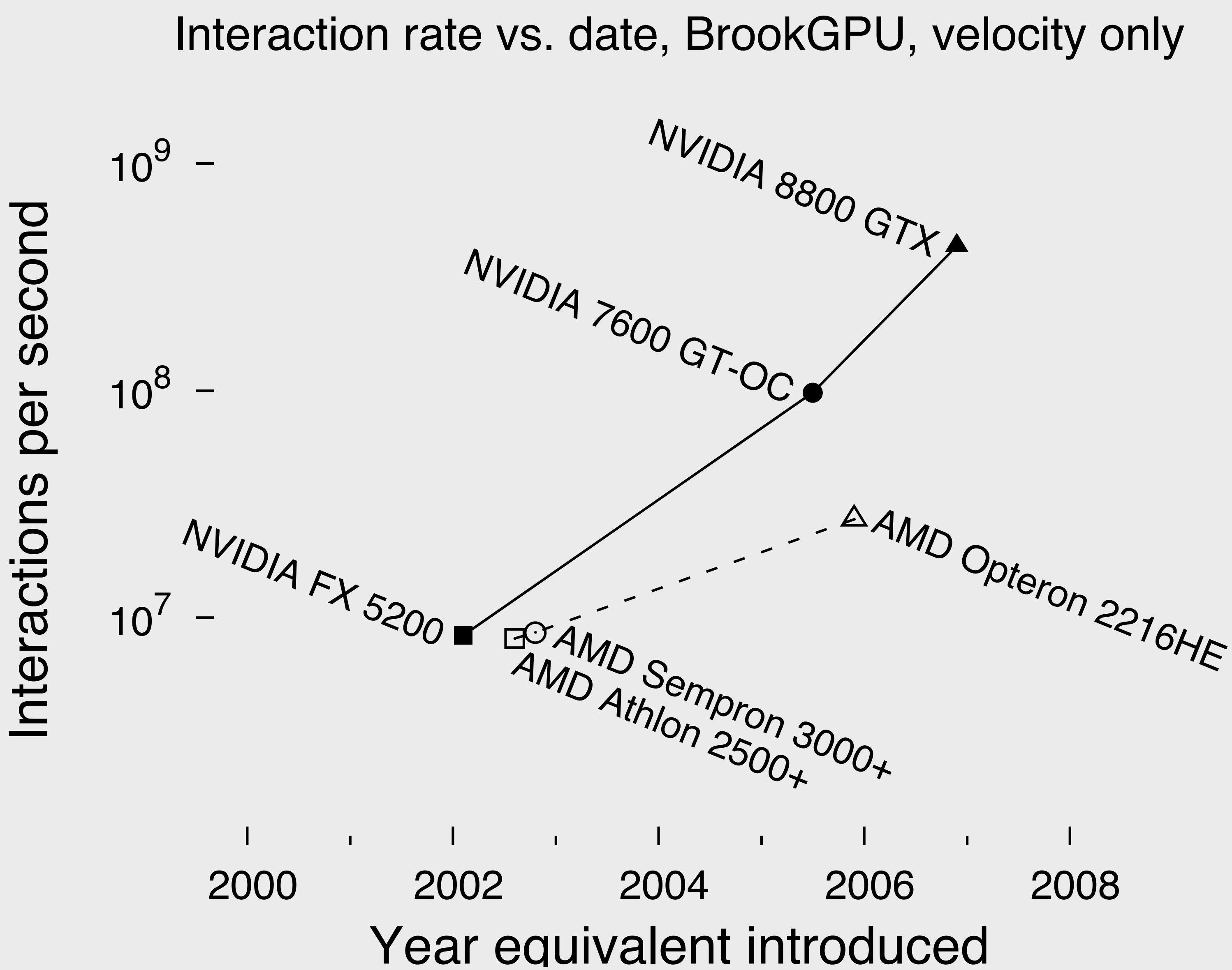
Conclusions

- Vortex particle methods adapt to hybrid CPU-GPU systems
- 140x speedup for direct summations on GPU
- 10x-15x speedup for GPU treecode velocity-finding
- 3.4x speedup for full dynamic timestep

Conclusions

- **GPU performance has increased rapidly...and should continue**



Future Work

- Reorganize to more efficiently use CPU & GPU
- Put VRM diffusion onto GPU
- Test on distributed-memory CPU-GPU clusters

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Thank you for your attention! Any questions?

mstock@applied-scientific.com