Recent advances in dynamic effects in OuroborosBEM

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OuroborosBEM

Microscopic MC simulation for particle transport in an electric field on GPUs

- Gases available: Ar, CO_2, N_2, CF_4, CH_4, iC_4H_{10}, O_2
- Interaction cross sections for mixture gases
- Electron anisotropy scattering
- Penning transfer probability
- 2 different integration algorithms: Euler or PEFRL (δt=25 fs)
- Signal generation through Ramo field maps
- Extraction of lots of observables (v_d, <E>, positions,...)
- Electric field calculation (static, dynamic, RF)

The field

- Calculated using a Boundary Element Method (mesh=surface elements)
  - unknowns: cell surface charge densities $V = Q\sigma$ (Q: $\int \frac{1}{4\pi\epsilon_0 r} dS$)
- Common behaviour at start (e.g. 12000 cells):
  1. Fill matrix Q ($\sim$100 ms)
  2. Matrix inversion Q^{-1} ($\sim$1.2 s)

Static option: once at the beginning of the simulation

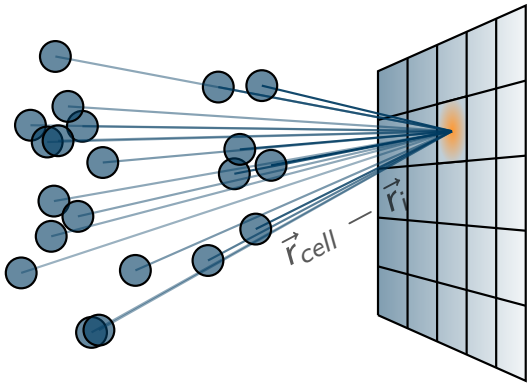
- Creates a field map and a geometry map (and Ramo field maps) at predefined grid points: $Q^{-1}V = \sigma \rightarrow \vec{Q}_{grid}\sigma = \vec{E}$, ($512^3$: $\sim$200s)

Dynamic option

- Every N step (N≠1: approximation) and at each particle position

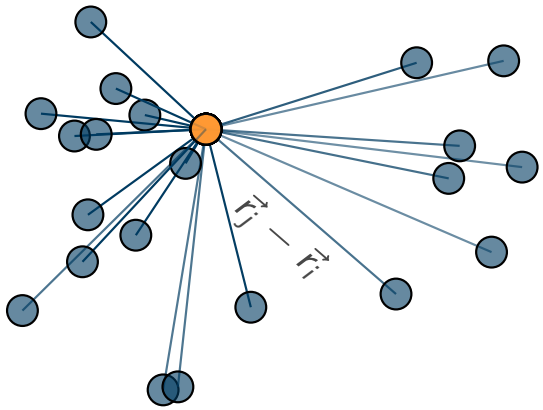
1. Change the potential of each cell
2. Calculate the influence of the particles on the cells:

$$V_{cell\,/\,i} = \sum_{i}^{N_{part}} \frac{1}{4\pi\varepsilon_0} \frac{q}{\parallel \vec{r}_{cell} - \vec{r}_i \parallel}$$



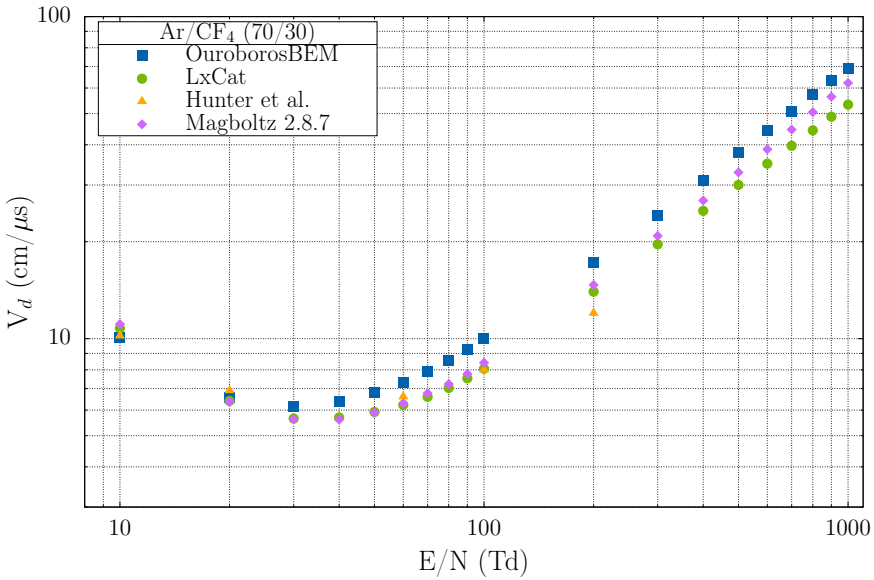
3. $Q^{-1}V = \sigma$
4. $\vec{Q}_{part}\sigma = \vec{E}$
5. Add the contribution of the particles on the field:

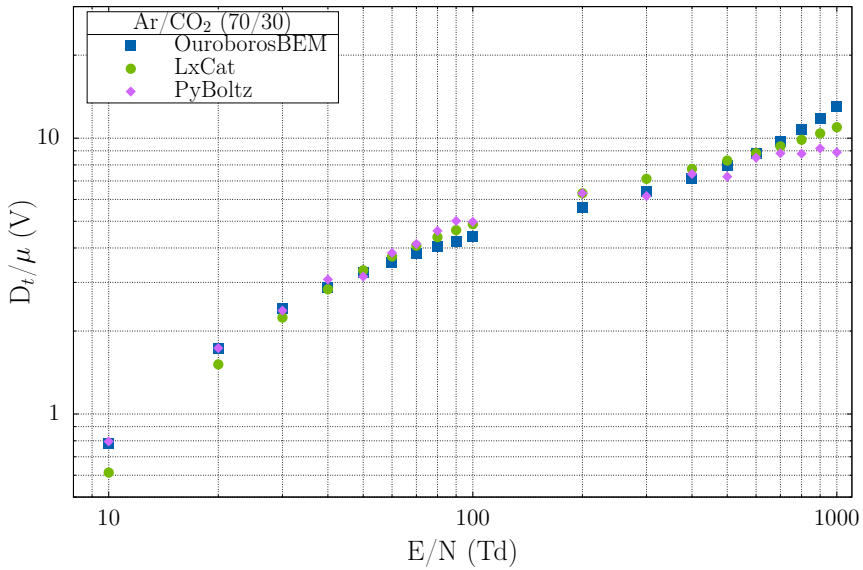
$$\vec{E}_i = \sum_{j,i\neq j}^{N_{part}} \frac{q^2}{4\pi\varepsilon_0} \frac{\vec{r}}{\parallel \vec{r}_i - \vec{r}_j \parallel^3}$$



Recent validation

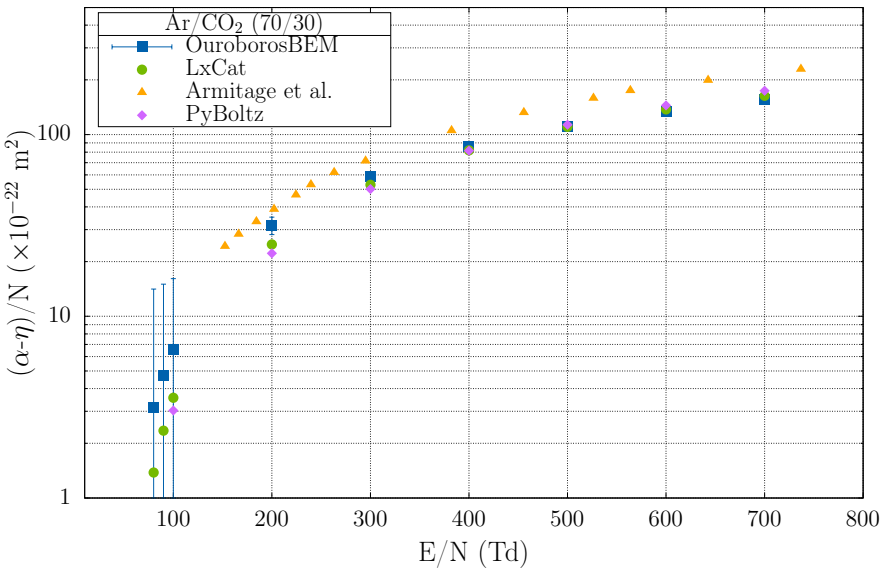
- Drift velocities and diffusion coefficient

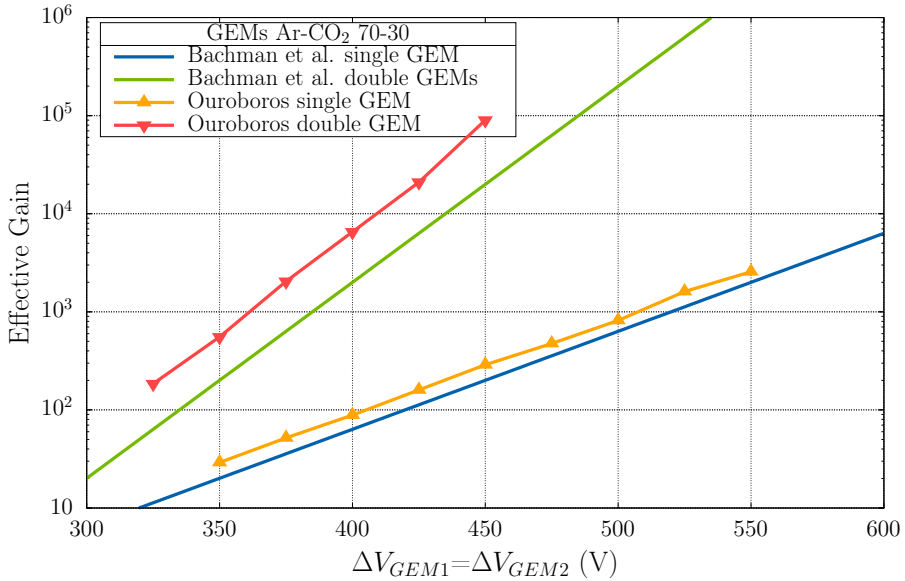




Recent validation

- First Townsend coefficient α and gas gain in GEMs ($r_{Penning} = 0.574$, Şahin et al. NIMA 768, 104-111, 2014)





Results are quite cross section dependant

What's new

Saving data

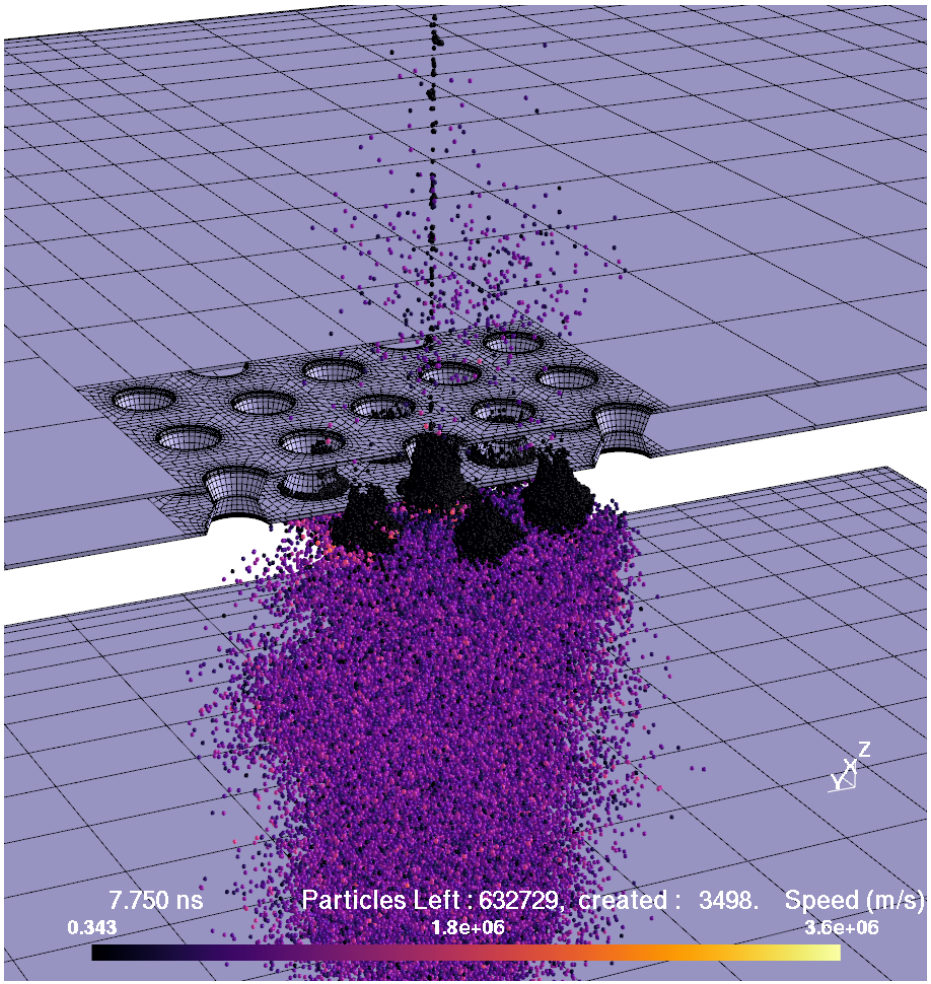
- Autosave time
- Escape time and restart from previous simulation

Speeding-up

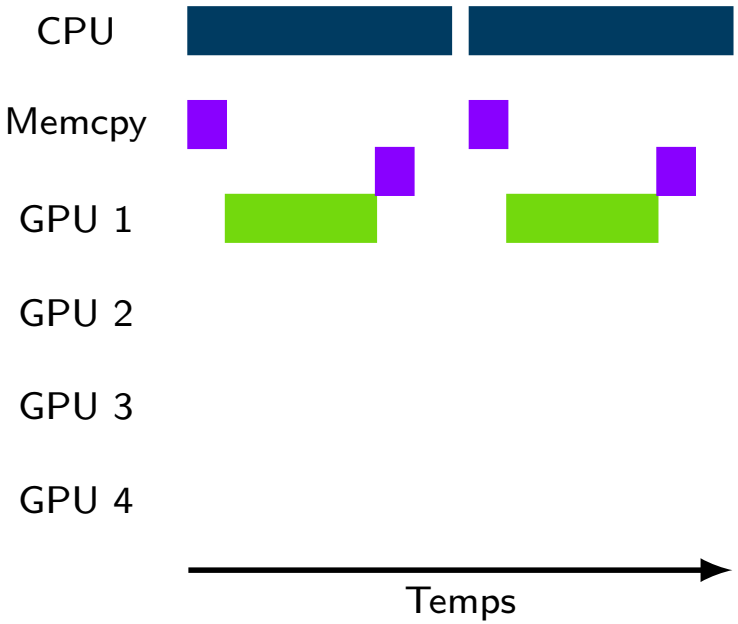
- Multi-GPUs
- Nearest neighbours algorithm

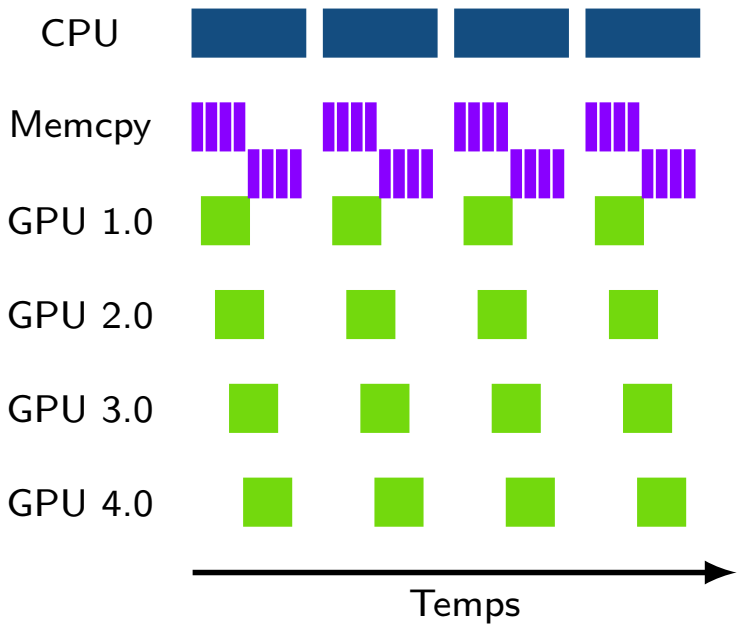
Physics

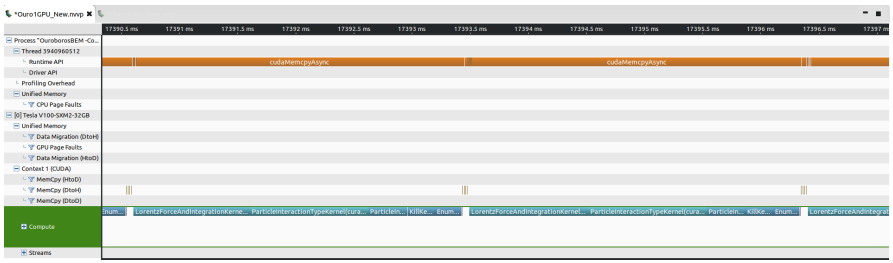
- Charging-up
- Microscopic ion transport
- Recombination

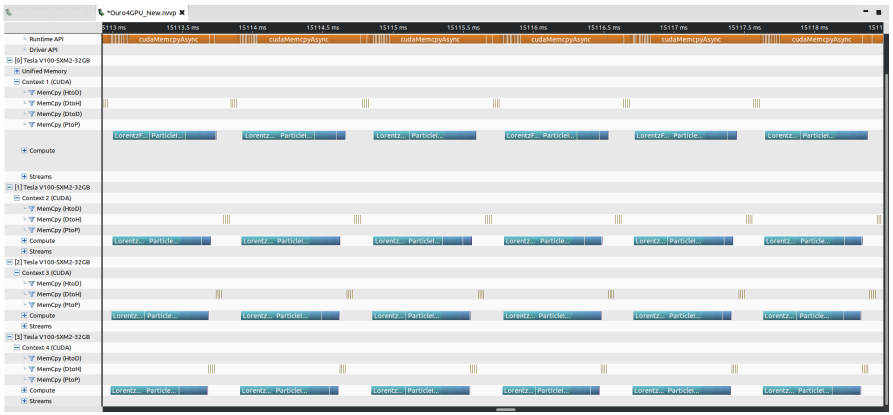


OuroborosBEM Multi-GPUs



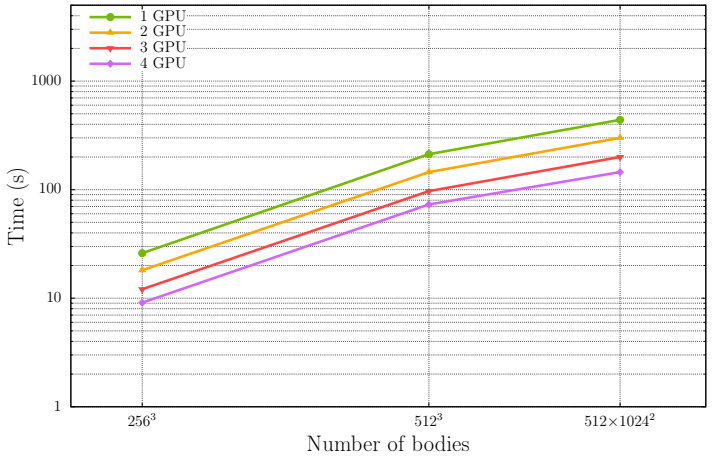






OuroborosBEM multi-GPUs

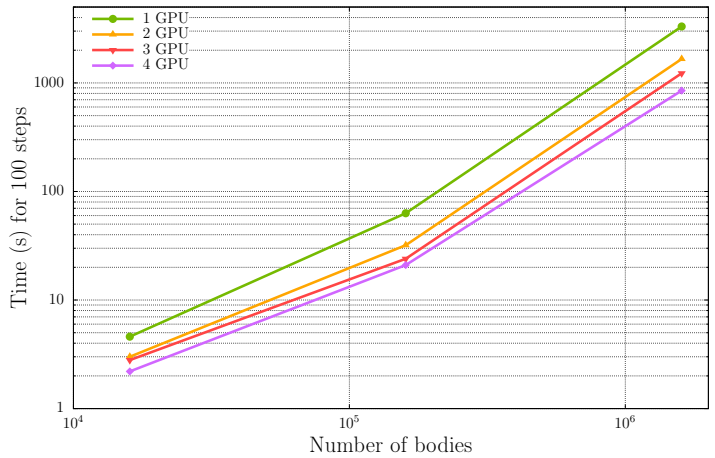
Static calculation time



# Map size	# GPUs 1	2	3	4
256^3	34 s	17 s	11 s	8 s
512^3	212 s	145 s	97 s	73 s
512×1024^2	1088 s	544 s	352 s	250 s

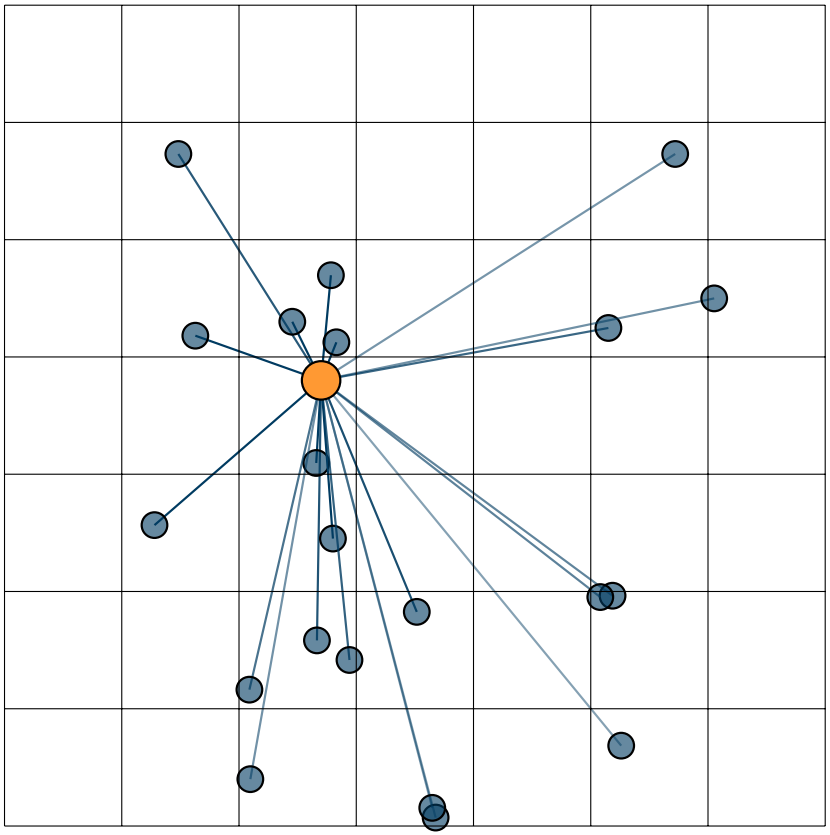
Dynamic calculation for 100 steps

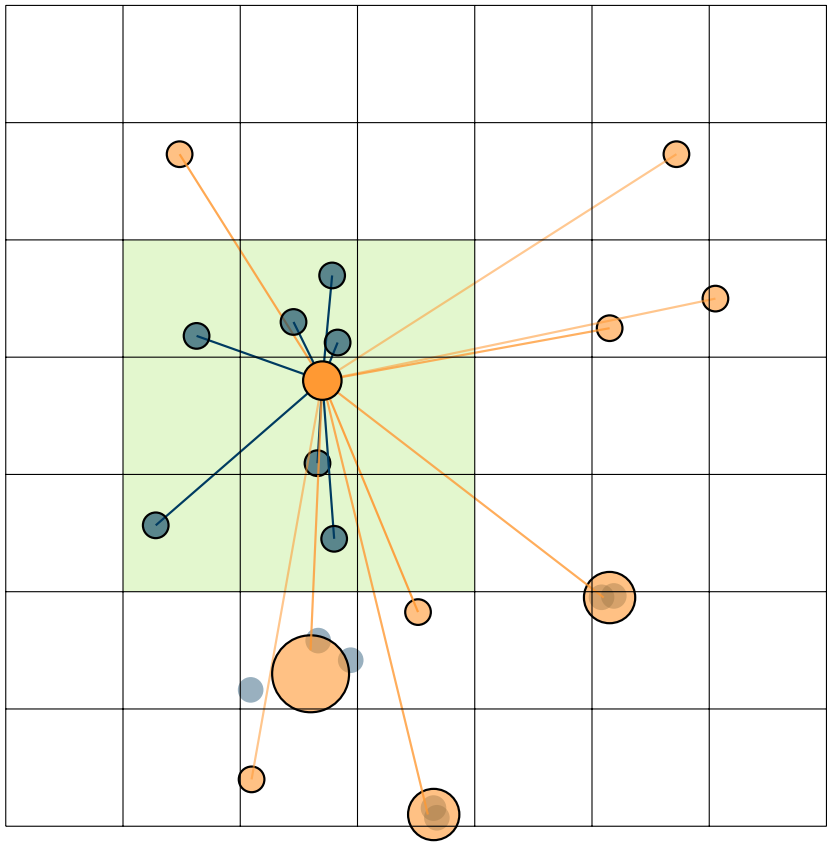
# bodies	# GPUs 1	2	3	4
16000	4,6 s	3 s	2,8 s	2,2 s
160000	63 s	32 s	24 s	21 s
1600000	3311 s	1661 s	1227 s	850 s



Calculating the N-Body problem

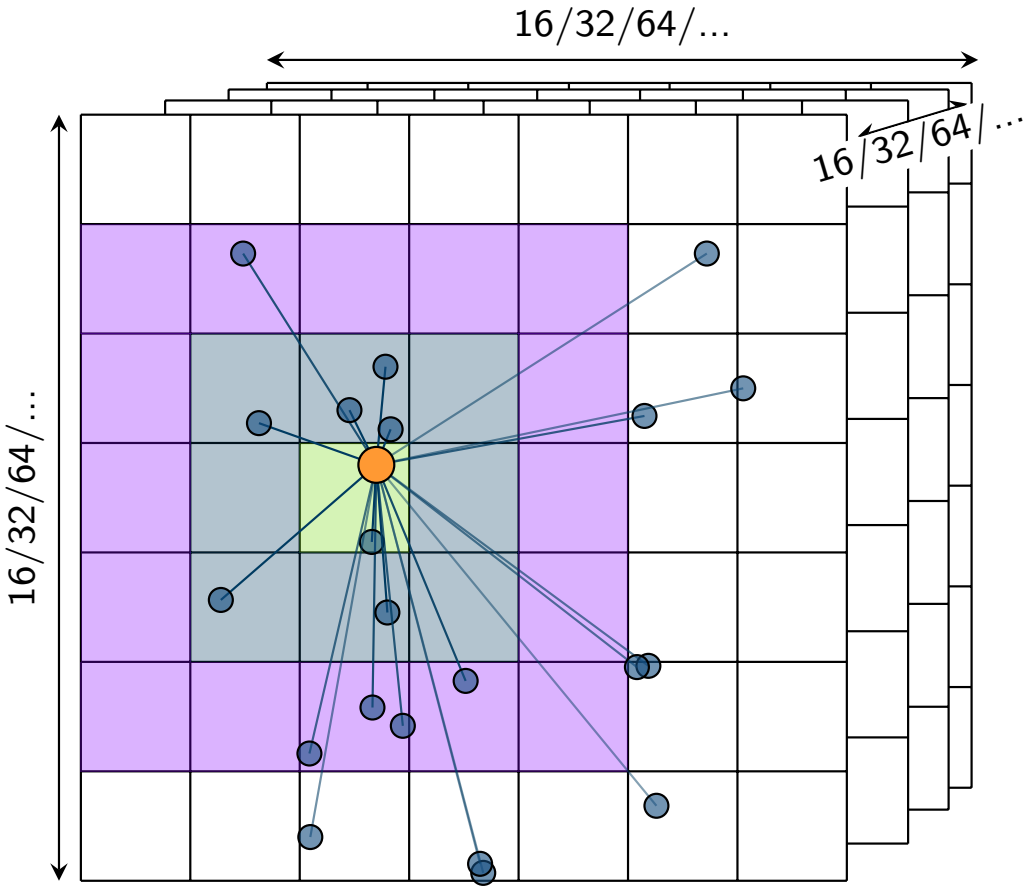
- Far field approximation: exact calculation only for the closest particles





Calculating the N-Body problem

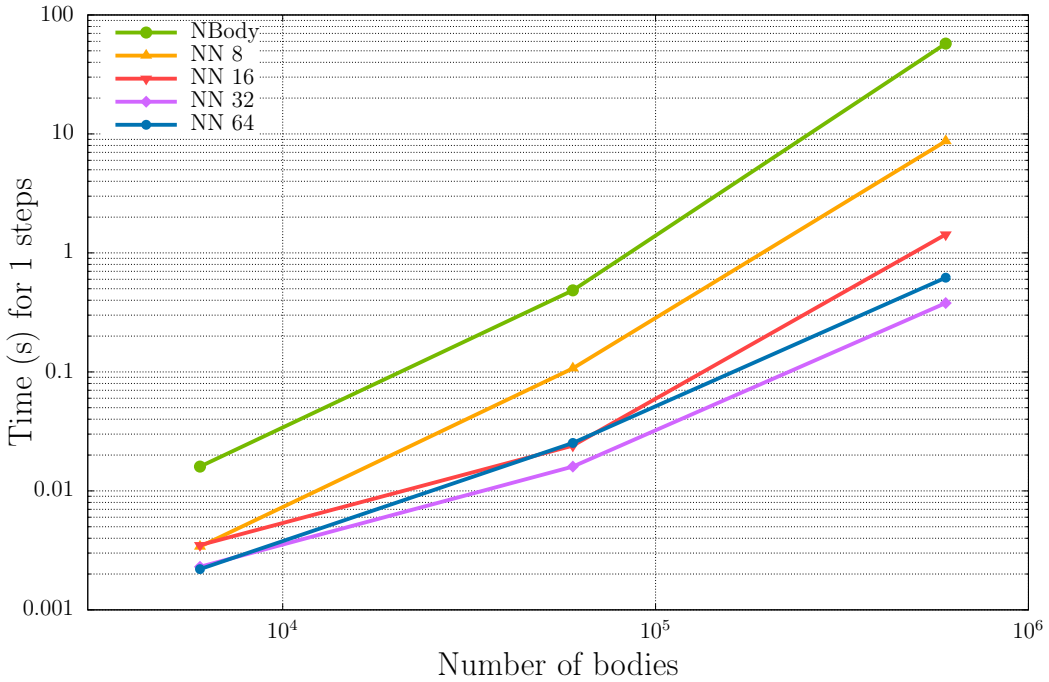
- 2 parameters: grid size and calculation order



OuroborosBEM: 'Nearest neighbours'

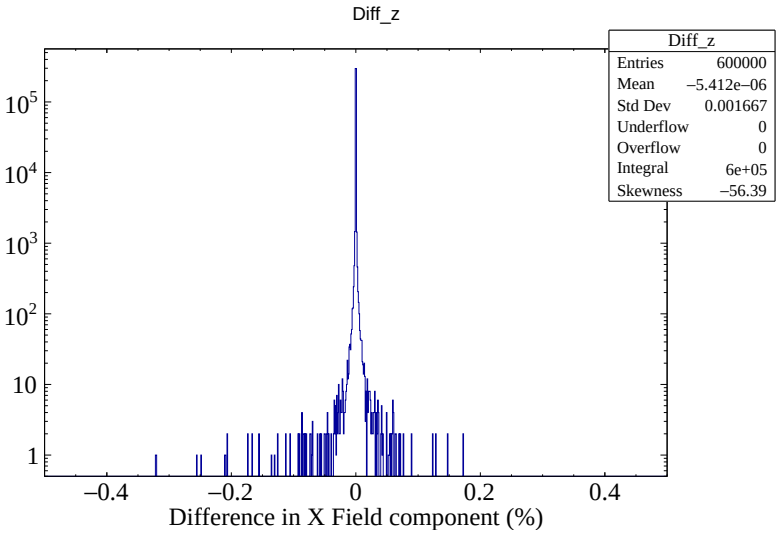
Grid size

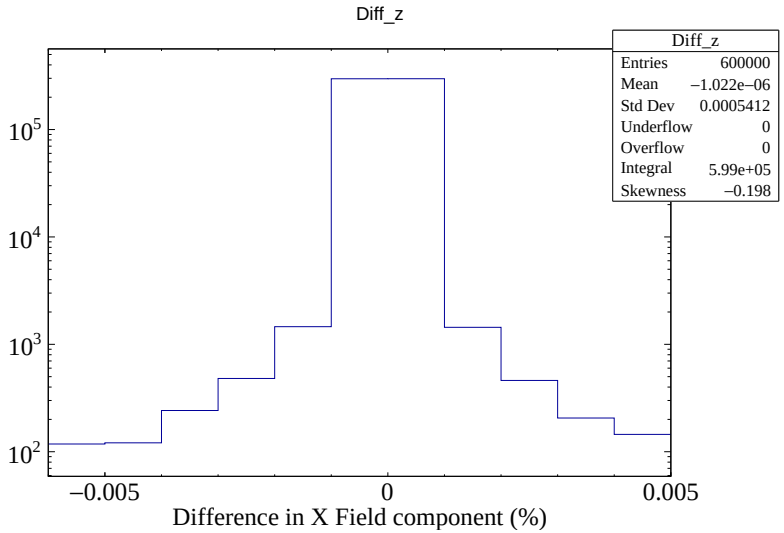
# bodies	NBody	# NN			
		8,8,8	16,16,16	32,32,32	64,64,64
6000	16 ms	3,4 ms	3,5 ms	2,2 ms	2,2 ms
60000	485 ms	107 ms	24 ms	16 ms	25 ms
600000	57,5 s	8,7 s	1,43 s	379 ms	619 ms



OuroborosBEM: 'Nearest neighbours'

Order, Relative differences compared to the exact calculation of the x component of the field (600000 particles, 32,32,32)



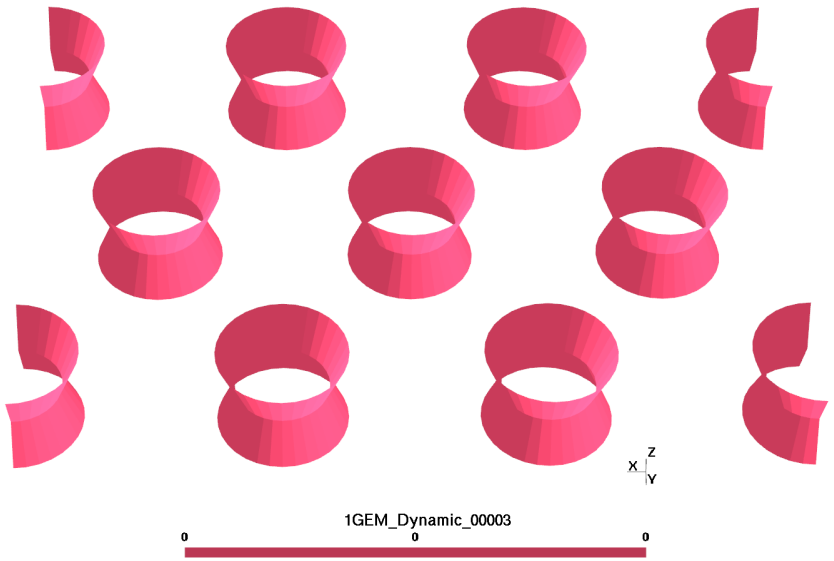


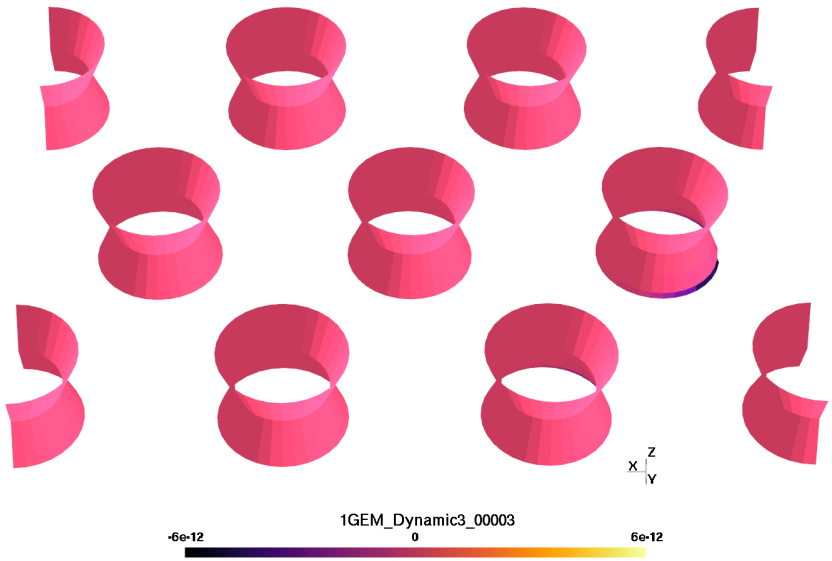
Order	Time	Interval : -0.5;0.5 (%)			Interval : -0.005;0.005 (%)		
	(1 step)	μ ($\times 10^{-6}$)	σ ($\times 10^{-3}$)	N (%)	μ ($\times 10^{-6}$)	σ ($\times 10^{-4}$)	N (%)
0	190 ms	15,0	9,2	99,7	-12,1	9,5	97
1	375 ms	-5,0	4,0	100	-3,24	6,36	99,4
2	1,02 s	-4,6	2,9	100	0.05	5,7	99,7
3	1,98 s	5,4	1,6	100	-1.02	5,4	99,8

Charging-up

Changing the dielectric cells surface charge densities $\sigma_{F,i}(t)$

- $\sigma_{F,i}(t + \Delta t) = \sigma_{F,i}(t) + \frac{1}{A_i} \sum_{p=1}^{\mathcal{N}_{p,i}} q_p$
- Delayed by 1 time step for efficiency purposes
- No evacuation for the moment
- Effect is obviously small for $\mathcal{N}_{p,i} < 1 \times 10^{5-6}$
- But can be increased using "Macro" particles





Towards full Monte Carlo calculations

Ion scattering cross sections

- $Ar^+ + Ar$ data (Phelps calculations) only
- Isotropic and back-scattering
- Same treatment in the code for electrons and ions

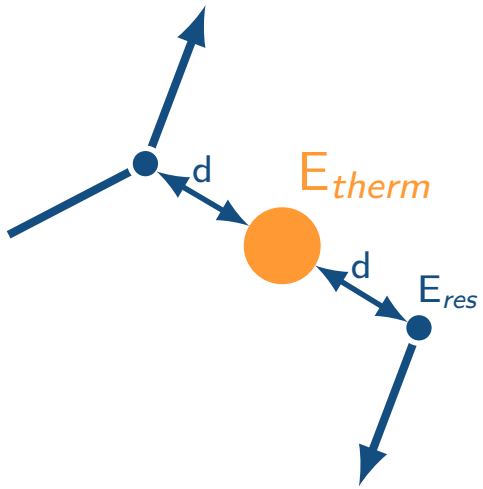
Dynamic microscopic calculations

- Knowledge of the distance between closest electrons and ions
- No difference between anions and cations (created through attachment) due to missing cross sections
- Possibility for recombination processes...

Recombination: Classical representation

1. Creating the electron/ion pair in the ionisation process

- Thermal energy of the ion (3/2kT)
- Electron residual energy $\sim$ Recoil energy
- Both electrons have opposite momentum in the c.m.
- Distance between the electron and ion from Coulomb barrier: $d = \frac{1}{4\pi\varepsilon_0}\frac{q}{E_{res}} \simeq 1.44\ \text{eV}\cdot\text{nm}/E_{res}$



Recombination: Classical representation

2. Inverse process for recombination

- Distance d is known during the 'Nearest neighbours' process
- If $d < \frac{1}{4\pi\varepsilon_0}\frac{q}{E_{ioni}}$, the particles recombine
- But what about their kinetic energies?
  - Can be large due to Coulomb attraction
  - Energy is above ionisation potential...
- If d is too small, might never recombine due to the time step (25 fs)...

3. Another approach?

- Statistical one: probability to recombine if certain conditions apply?
- Semi-quantum one: which calculations and at what cost?

Still to be tested and validated with data (but which ones?)

Perspectives

What's next?

- A valid recombination process
- Charging-up functions
- "Resistive materials" to evacuate charges (useful in μ-RWell, MicroMegas...)
- NURBS: reducing the number of cells and increase the precision
- Ideally: as much cross-sections as possible