Simulation of a many-particle system using space partitioning

Roald Frederickx, Kasper Meert:

Inleiding

Implementation

Performance

Toepassingen

Maxwell-Boltzmann

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2 Implementatie

3 Performance

- 4 Toepassingen
 - Maxwell-Boltzmann

Relevantie

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Toepassingen Maxwell-Boltzman Veel fysische systemen te modelleren door interagerende deeltjes

Bijvoorbeeld

- Ideaal gas
- Elektronen in metaal
- Maxwell-Boltzmann verdeling fi ffi fl
- Adsorptie
- Diffusie
- Warmtegeleiding

Enkel korte-afstand interactie!

Simulatie — Naïef

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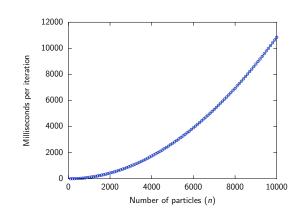
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Implementatie

Toensssing

■ Elk paar apart bekijken

- $O(n^2)$
- Veel overbodig werk



Oplossing: Space partitioning

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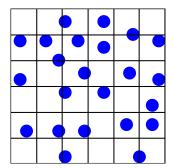
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Toepassingen Maxwell-Boltzmann

- Ruimte onderverdelen in "dozen"
- n deeltjes
- x deeltjes per doos
- n/x dozen
- Complexiteit $O(n/x \cdot x^2) = O(nx) = O(n)$



Implementatie

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Toepassingen Maxwell-Boltzmann

- Programmeertaal: C
- Harde bollen
- Elastische botsingen
 - A posteriori
 - Backtracking
- "Doos" = lijst

Testen op botsingen

- Binnen eigen doos
- Buurdozen

Wereld vullen

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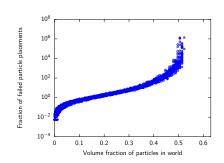
Toepassingen

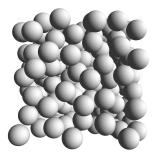
■ Genereer willekeurige positie

Zolang botsing: probeer opnieuw

Volumefractie gestapelde bollen:

- Maximaal \approx 74% op een regelmatig rooster
- Willekeurig ≈ 63% mits "schudden"
- Ons algoritme $\approx 52\%$





Simulation of

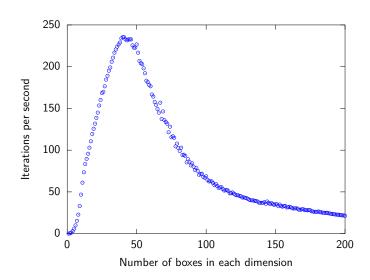
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Simulation of

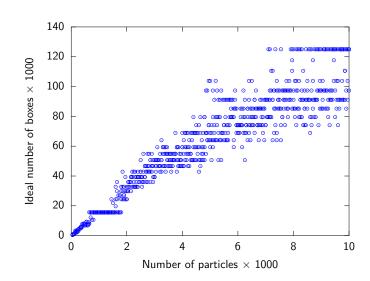
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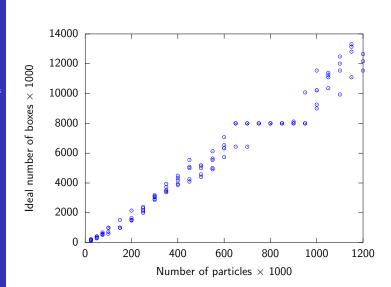
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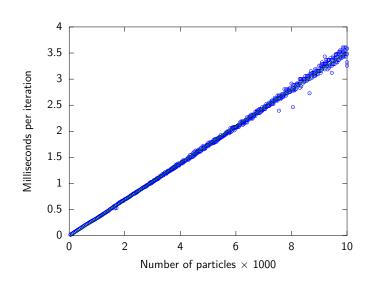
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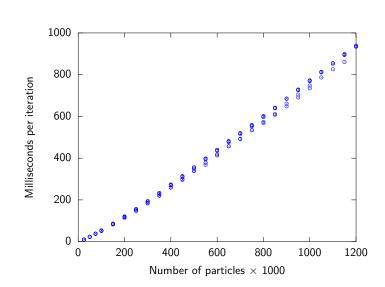
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Performance conclusie

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- ~ 10 dozen per deeltje
- $O(n^2) \rightarrow O(n)$
- lacksquare 5 jaar ightarrow 1 seconde

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Maywell Reltament