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# Using Ray Tracing to Model Thermal Radiation in LIGGGHTS

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# Outline

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# Model - Depiction

A sketch of ray tracing

- Red sphere emits a ray that is reflected twice and heats up blue sphere.
- Blue sphere emits ray that hits background and leads to heat transfer from the background.
- Gray arrows are normal vectors.

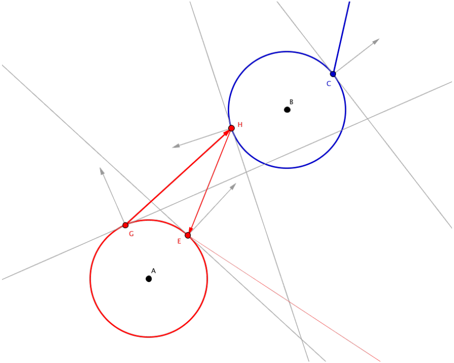


Figure 1: Depiction of radiation of two spheres.

# Model - Description
## Assumptions

based on the idea of raytracing and Stefan Boltzmann's law.

### Simplifying Assumptions

- homogeneous temperature of particles:

$$\text{rays originate on points } \sim U(\text{surface of particle})$$

- instantaneous heat transfer within particle (particle has *one* temperature)
- purely diffuse surfaces (for the moment)
  - angle of reflection $\sim U(-\pi/2, \pi/2) \times U(-\pi/2, \pi/2)$
  - no refraction
- emissivity is constant across all wavelengths
- correctness of Stefan Boltzmann's law
- constant background radiation

# Model - Description

## Algorithm for One Timestep

for each particle $i$:

- generate random point on particle
- generate random direction (pointing to outside of particle $i$)
- calculate heat flux using Stefan Boltzmann's law: $\dot{Q}_i = \epsilon_i \sigma A_i T_i^4$
- decrease heat flux of particle $i$ by $\dot{Q}_i$
- trace ray for intersections with other particles
- if (intersection with particle $j$):
  - transfer absorbed part of heat: $\dot{Q}_i \epsilon_j$
  - generate random direction (that points outside of particle $j$)
  - shoot new reflection ray with $\dot{Q}_j = (1 - \epsilon_j)\dot{Q}_i$ (recursively, up to depth $N$)
- else (assume background radiation):
  - increase heat flux of particle $i$ by $\epsilon_i \sigma A_i T_{\text{background}}^4$

# Model - Description
## Formal Description - Definitions

**Definition 1 (used sets)**

*Let $I$ be the set of particles, $\varnothing$ the background with temperature $T_\varnothing$ and $U := \{\varnothing, I\}$.*

**Definition 2 (general symbols)**

*For a particle $i$ let $T_i$ denote its temperature, $A_i$ its surface area and $\epsilon_i$ its emissivity. Furthermore let $\sigma$ be Stefan Boltzmann's constant.*

**Definition 3 (relation symbols)**

- $\forall i \in I, j \in U : i \rightsquigarrow j$
  $\iff$ *a ray that was cast from $i$ hit or has been reflected to $j$.*
- $\forall i, k \in I, j \in U : i \overset{k}{\rightsquigarrow} j$
  $\iff$ $i \rightsquigarrow j \wedge$ *the ray from $i$ was reflected via $k$.*
- $\forall i \in I, j \in U : N_{i \rightsquigarrow j}$ *is the number of reflections from $i$ to $j$*

# Model - Description

## Formal Description - Model

Using Iverson bracket notation and definitions 1, 2 and 3 the heat flux of a particle $i \in I$ is in this model defined as follows:

### Heat Flux of Particle $i \in I$

$$
\begin{aligned}
\dot{Q}_i := & -\epsilon_i \sigma A_i T_i^4 && (1) \\
& + \epsilon_i \sum_{\substack{j \in I \\ j \rightsquigarrow i}} \Big( \epsilon_j \sigma A_j T_j^4 \prod_{\substack{k \in I \\ j \overset{k}{\rightsquigarrow} i}} (1 - \epsilon_k) \Big) && (2) \\
& + [i \rightsquigarrow \varnothing] \epsilon_i \sigma A_i T_\varnothing^4 \prod_{\substack{k \in I \\ i \overset{k}{\rightsquigarrow} \varnothing}} (1 - \epsilon_k) && (3) \\
& + \epsilon_i \sigma A_i T_i^4 \prod_{\substack{j,k \in I \\ N_{i \rightsquigarrow j} > N_{\max} \vee \prod_{i \overset{k}{\rightsquigarrow} j} (1 - \epsilon_k) < 0.001}} (1 - \epsilon_k) && (4)
\end{aligned}
$$

# Model - Description

## Formal Description - Explanation

- (1): Heatloss due to cooling

$$-\epsilon_i \sigma A_i T_i^4$$

- (2): Particle to particle heat transfer due to radiation (including reflection)

$$+\epsilon_i \sum_{\substack{j \in I \\ j \rightsquigarrow i}} \left( \epsilon_j \sigma A_j T_j^4 \prod_{\substack{k \in I \\ j \overset{k}{\rightsquigarrow} i}} (1 - \epsilon_k) \right)$$

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# Model - Description

## Formal Description - Explanation

- (3): Background radiation

$$+[i \rightsquigarrow \varnothing]\epsilon_i \sigma A_i T_\varnothing^4 \prod_{\substack{k \in I \\ i \overset{k}{\rightsquigarrow} \varnothing}} (1 - \epsilon_k)$$

- (4): Residuum that arises due to cut-off of possibly infinite geometric series of reflections

$$+\epsilon_i \sigma A_i T_i^4 \prod_{\substack{j,k \in I \\ N_{i \rightsquigarrow j} > N_{\max} \vee \prod_{i \overset{k}{\rightsquigarrow} j} (1-\epsilon_k) < 0.001}} (1 - \epsilon_k)$$

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## Formal Description - Explanation

- (3): Background radiation

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# Outline

# Framework

LIGGGHTS allows to integrate scalar and vectorial properties.
e.g. initial temperature at $t_0$ + heat flux $\rightsquigarrow$ temperature at $t_1$

$\Longrightarrow$ suffices to calculate radiative heat transfer, integration is handled by LIGGGHTS

# Outline

# Usage of neighbor-lists

Don't check all particles for each ray.

1. Check all neighbors of emitting particle
2. Walk the neighbor-list-bins in the respective direction

# Usage of neighbor-lists
## Example

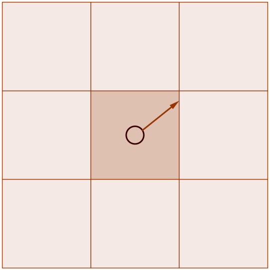


Figure 2: Check atoms of full stencil

Check for intersections, then find next central bin.

# Usage of neighbor-lists

## Example

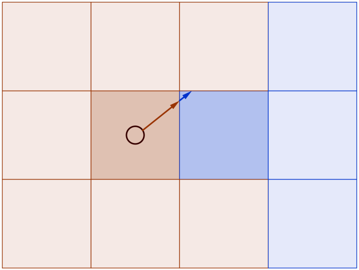


Figure 3: Check particles in new bins only (light blue)

Check for intersections, then find next central bin.

# Usage of neighbor-lists

## Example

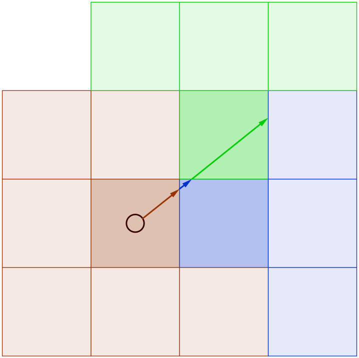


Figure 4: Check particles in new bins only (light green)

Check for intersections, then find next central bin.

# Usage of neighbor-lists
## Example

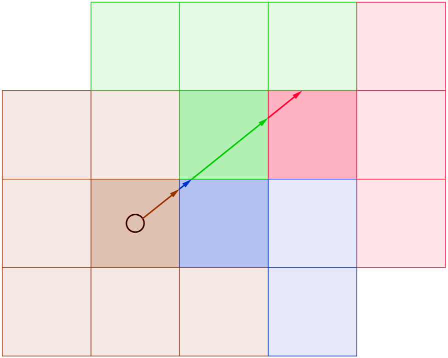


Figure 5: Check particles in new bins only (light red)

Check for intersections, then find next central bin.

# Outline

2 Implementation Details
- Usage of neighborlists
- Parallelization

# Parallelization

Heat transfer obeys inverse square law, thus we can

- introduce *maximum radiation-distance* to ignore “negligible” long distance contributions
- use maximum radiation-distance as “force” cutoff (`cutghost`) of radiation fix
- invoke forward / backward communication of heat-flux; use LIGGGHTS built-in parallelism

# Outline

# Qualitative Correctness

Bulk-behavior of a box of particles

- temperature adjusts to surrounding temperature
- corners cool off faster then surfaces
- visible temperature gradient within the bulk (inside: hot, outside: cools)

# Quantitative Correctness

Overview

- radiative cooling of a single sphere
  - temperature after a certain time
  - comparison with direct forward Euler integration of Stefan Boltzmann's law

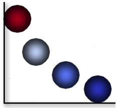


Figure 6: Radiative cooling of a single sphere.

- radiative heat transfer between two large, parallel planes
  (see [1], p. 821, Example 2)

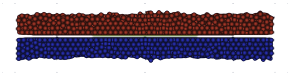


Figure 7: Radiative heat transfer between two parallel planes.

1 *VDI Wärmeatlas*, vol. 7, Verein Deutscher Ingenieure VDI-Gesellschaft Verfahrenstechnik und Chemieingenieurwesen (GVC), (german), 1994

# Quantitative Correctness

## Radiative Cooling of a Single Sphere - Results

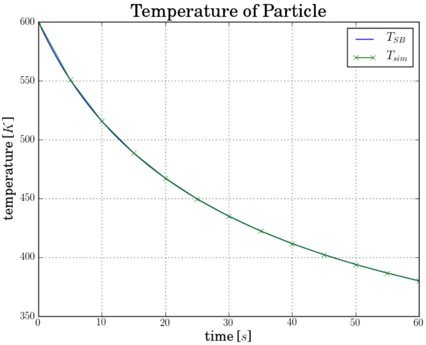



Figure 8: Temperature of integrated Stefan Boltzmann law vs. simulation using our radiation model.

$\Longrightarrow$ Model represents Stefan Boltzmann's law for a single particle.

# Quantitative Correctness

## Two Parallel Planes - Analytical Setup

Setup of the analytical solution:

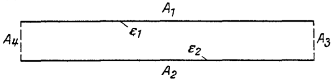



Figure 9: Setup of solution [1]

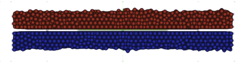


Figure 10: Radiative heat transfer between two parallel planes.

Analytical representation of heat transfer for this setup:

$$\dot{Q} = \frac{\sigma A}{\frac{1}{\epsilon_1} + \frac{1}{\epsilon_2} - 1} \cdot (T_1^4 - T_2^4)$$

- Simplification: No interaction with environment, no heat is lost due to cooling.
- Exaggerated heat conduction within the plates


1 *VDI Wärmeatlas*, vol. 7, Verein Deutscher Ingenieure VDI-Gesellschaft Verfahrenstechnik und Chemieingenieurwesen (GVC), (german), 1994

# Quantitative Correctness

## Two Parallel Planes - Results

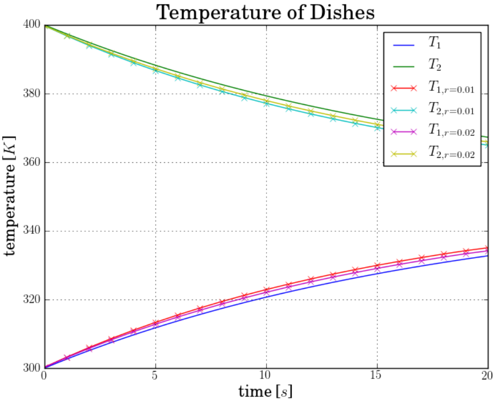



Figure 11: Temperature of both plates for 20 seconds and varying Radius.

# Quantitative Correctness

Two Parallel Planes - Results Explained

Small error of about 1% after 20 seconds, due to

- Grey particles (area correction calculated for black only)
- differing surface structure of flat planes vs. particulate planes.

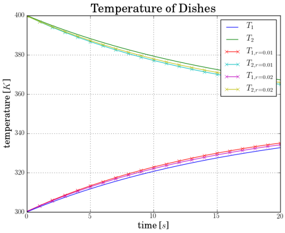
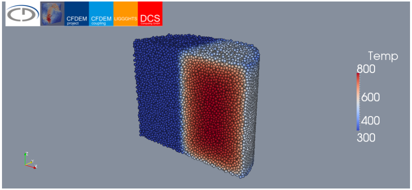



Figure 12: Temperature of both plates.

# Outline

# Examples

## Radiative Cooling of Particle Cylinder




Animation 1: Slice of particle-bed.

Simulation of radiative heat transfer of 110.000 particles on 16 cores.

- Particle radius: 2mm
- Cylinder:
  - Diameter: 70cm
  - Height: 2.8m
  - Vol. Frac.: 30%
- Walltime: 38 h
- CPUtime: 608 h
- simulated realtime: 25 sec

# Literature / Discussion

[1] *VDI Wärmeatlas*, vol. 7, Verein Deutscher Ingenieure VDI-Gesellschaft Verfahrenstechnik und Chemieingenieurwesen (GVC), (german), 1994.

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# Thank you.
# Questions?

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