# 多体問題専用計算機"GRAPE-6"を用いた微小スケールのプラズマの計算機実験

## Micro-scale Plasma Simulation Using Numerical Calculation Accelerator "GRAPE-6"

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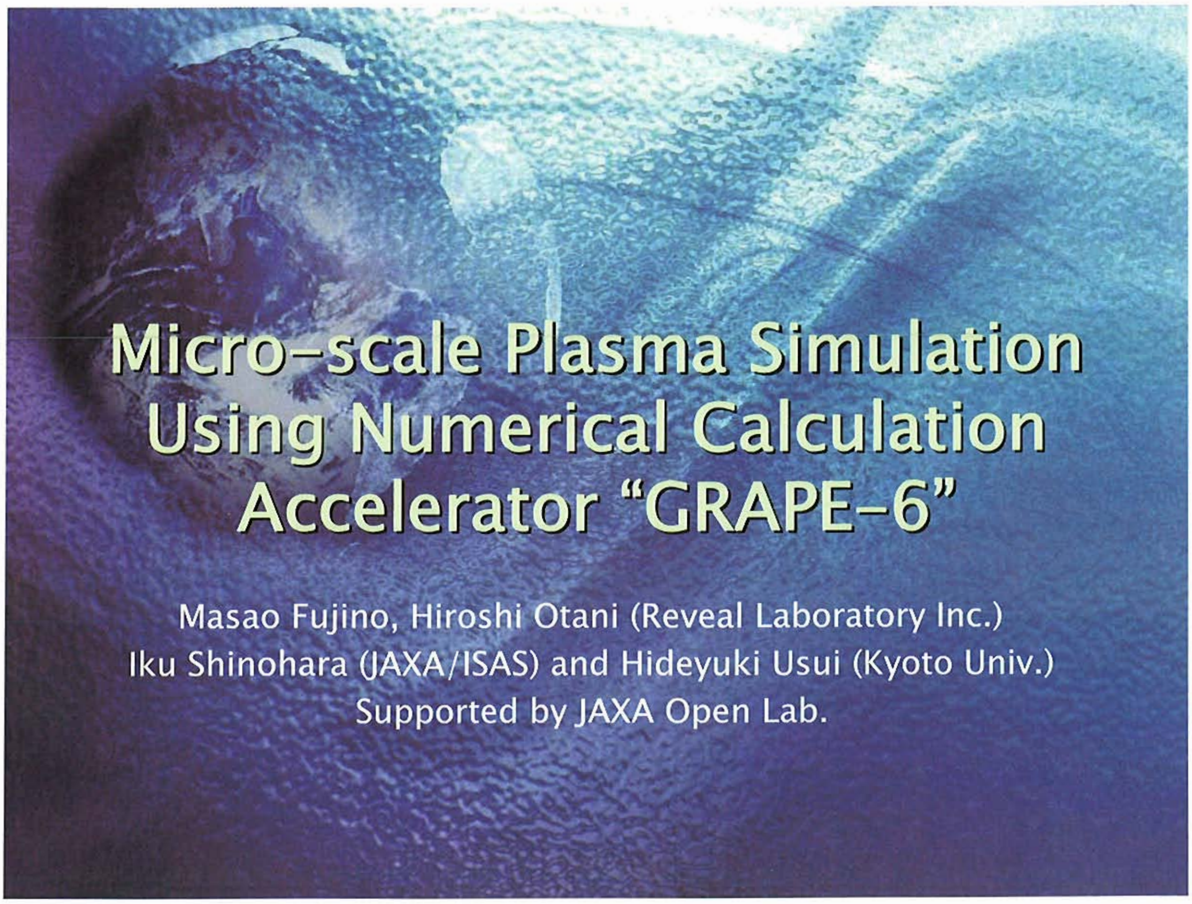
現在のプラズマの主要な計算機実験法である PIC 法では、デバイ長よりも小さいスケールでの実験はその原理上困難となっています。私達は、今までの手法では計算機実験を行うことのできなかった微小スケールでのプラズマの計算機実験の手法を確立し、プラズマのデバイ長が宇宙機と比べて大きくなる深宇宙においての宇宙機の性能評価法を確立することを目標として研究・開発を行っています。具体的には、天文の分野で使われている多体問題専用計算機"GRAPE-6"を用いて、プラズマ内の粒子にかかるクーロン力を直接計算することにより、プラズマ内の粒子の動きを直接追う純粋な粒子法の確立を目指しています。プラズマ内の粒子の動きを直接に追う場合、プラズマに含まれる粒子の数が膨大であるため、計算時間も膨大になってしまいます。そこで、"GRAPE-6"の粒子間の相互作用を高速に計算する能力に注目し、現実的な時間内での粒子法によるプラズマの計算機実験を行いたいと考えております。現在、その第1段階として、"GRAPE-6"を用いた粒子法のラングミュアプローブモデルによる検証を行っています。

この研究は JAXA オープンラボによる支援を受けて行われています。


図1 多体問題専用計算機 "GRAPE-6"


Micro-scale Plasma Simulation Using Numerical Calculation Accelerator "GRAPE-6"
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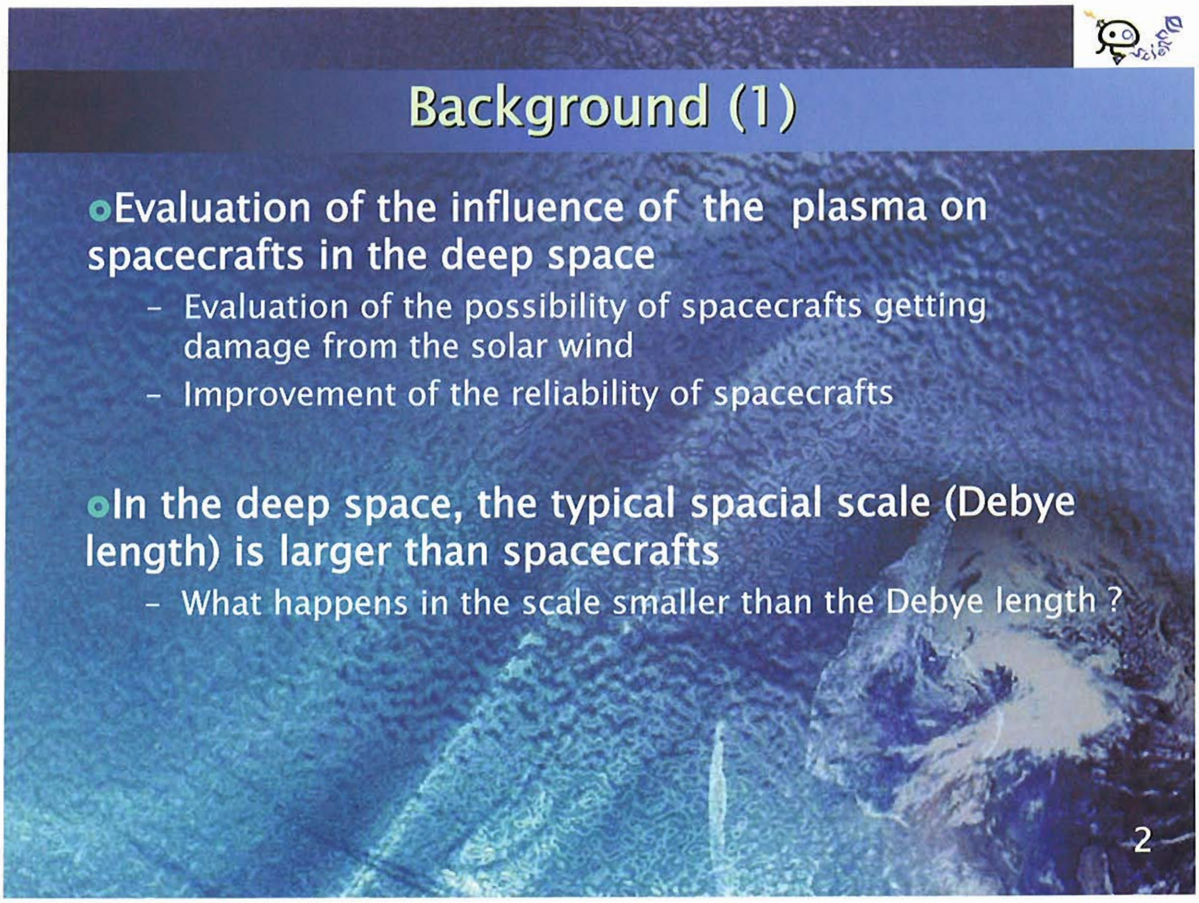
Supported by JAXA Open Lab.


Background (1)
Evaluation of the influence of the plasma on spacecrafts in the deep space
- Evaluation of the possibility of spacecrafts getting damage from the solar wind
- Improvement of the reliability of spacecrafts
In the deep space, the typical spacial scale (Debye length) is larger than spacecrafts
- What happens in the scale smaller than the Debye length ?
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## Background (2)

- PIC (Particle In Cell) method (Traditional)
  - Assumption of the scale larger than the Debye length
- Particle method (This work)
  - It can be used for the simulation whose scale is equal to or smaller than the Debye length
  - It is needed to calculate the Coulomb force on every particles from every other particles

→The calculation time will be longer

→Shorten the calculation time by using "GRAPE-6"

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## GRAPE-6 –Functionality

- Calculation of potential, acceleration and jerk
  - In the case of the same time step interval
  - Input parameters are masses, positions and velocities of the particles
  - They are most dominant in N-body simulations. Typically, their calculation costs are O(N^2)

$$\phi_i = \sum_{j \neq i} -Gm_j \frac{1}{\left(r_{ij}{}^2 + \varepsilon^2\right)^{1/2}}$$

$$\boldsymbol{a}_i = \nabla \phi_i = \sum_{j \neq i} Gm_j \frac{\boldsymbol{r}_{ij}}{\left(r_{ij}{}^2 + \varepsilon^2\right)^{3/2}}$$

$$\dot{\boldsymbol{a}}_i = \sum_{j \neq i} Gm_j \left[ \frac{\boldsymbol{v}_{ij}}{\left(r_{ij}{}^2 + \varepsilon^2\right)^{3/2}} - 3\left(\boldsymbol{v}_{ij} \cdot \boldsymbol{r}_{ij}\right) \frac{\boldsymbol{r}_{ij}}{\left(r_{ij}{}^2 + \varepsilon^2\right)^{5/2}} \right]$$

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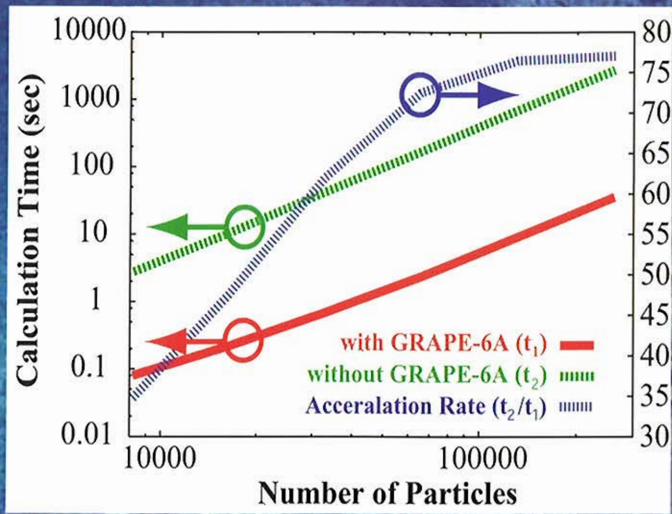
## GRAPE-6 –Performance

- A few ten times faster than the Intel Pentium 4 3.0GHz
  - In the case it calculates all interactions without any approximation

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## GRAPE-6 –Architecture (1)

- Pipelines dedicated for the gravity calculation
  - A kind of Digital Signal Processor (DSP)
  - Specialized in potential, acceleration and jerk calculation
  - Additionally, neighboring particle detection calculation
- Effective memory transfer
  - Minimized instruction transfer to the GRAPE-6 processor
  - 1 real pipeline acts as 8 virtual pipelines by time division
- Accelerator board works by calling the C/Fortran Functions (API)
  - After sending data to the GRAPE-6 board, receiving data of calculation result from it

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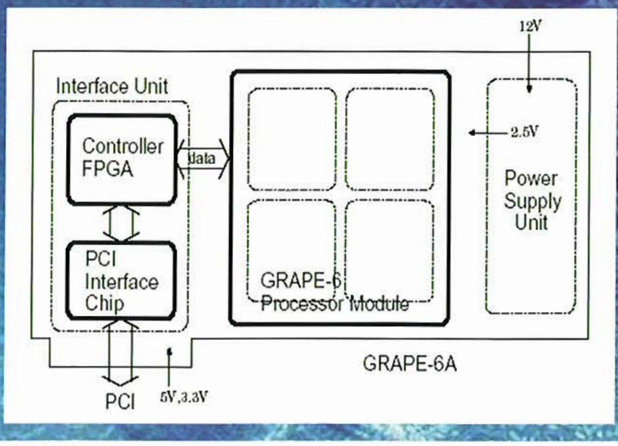
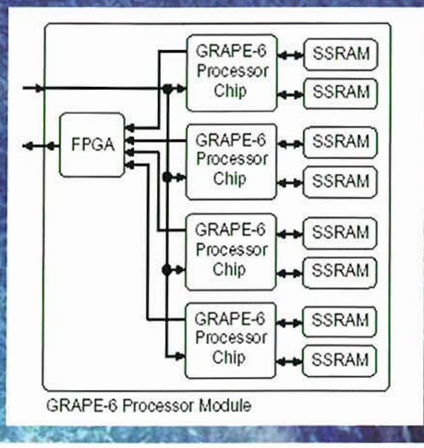
# GRAPE-6 –Architecture (2)

- GRAPE-6 processor
  - 0.25um process, 100MHz clock frequency
- SRAM
  - Stores 271,444 particles at the maximum (16MB x 2)
- FPGA
  - One is for the controller, the other is for reduction operation

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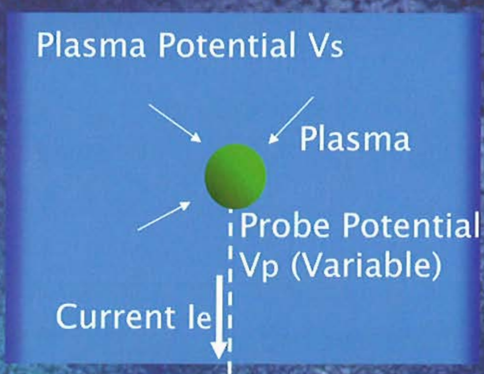
# Simulation Target –Langmuir Probe




- Change the probe potential Vp and measure the current Ie
- From the relationship between Vp and Ie, estimate the electron temperature Te and density Ne
- Compare the estimated Te and Ne to the value of those initially assumed

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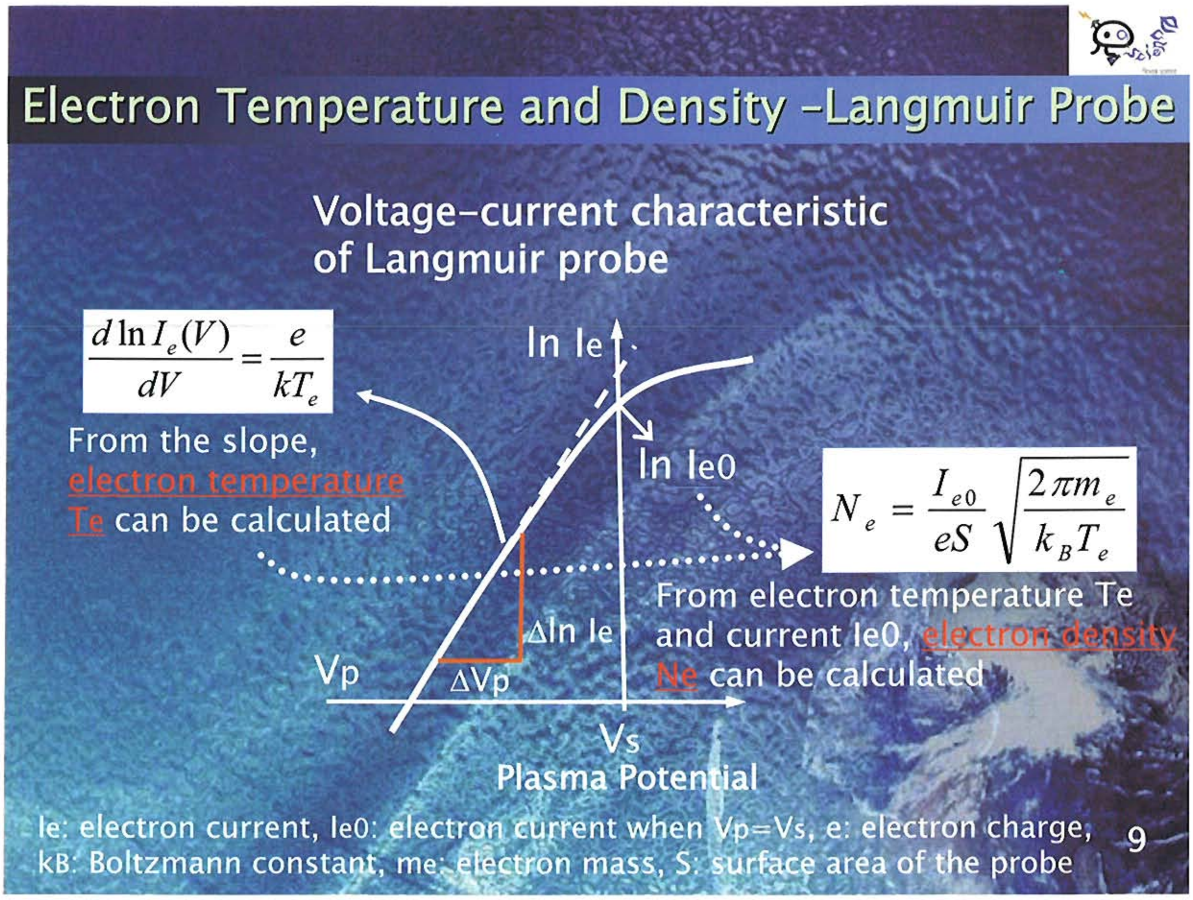
Electron Temperature and Density -Langmuir Probe
Voltage-current characteristic of Langmuir probe
$\frac{d \ln I_e(V)}{dV} = \frac{e}{kT_e}$
From the slope, electron temperature Te can be calculated
ln Ie
ln Ie0
$N_e = \frac{I_{e0}}{eS}\sqrt{\frac{2\pi m_e}{k_B T_e}}$
From electron temperature Te and current Ie0, electron density Ne can be calculated
ΔIn Ie
Vp
ΔVp
Vs
Plasma Potential
Ie: electron current, Ie0: electron current when Vp=Vs, e: electron charge, kB: Boltzmann constant, me: electron mass, S: surface area of the probe
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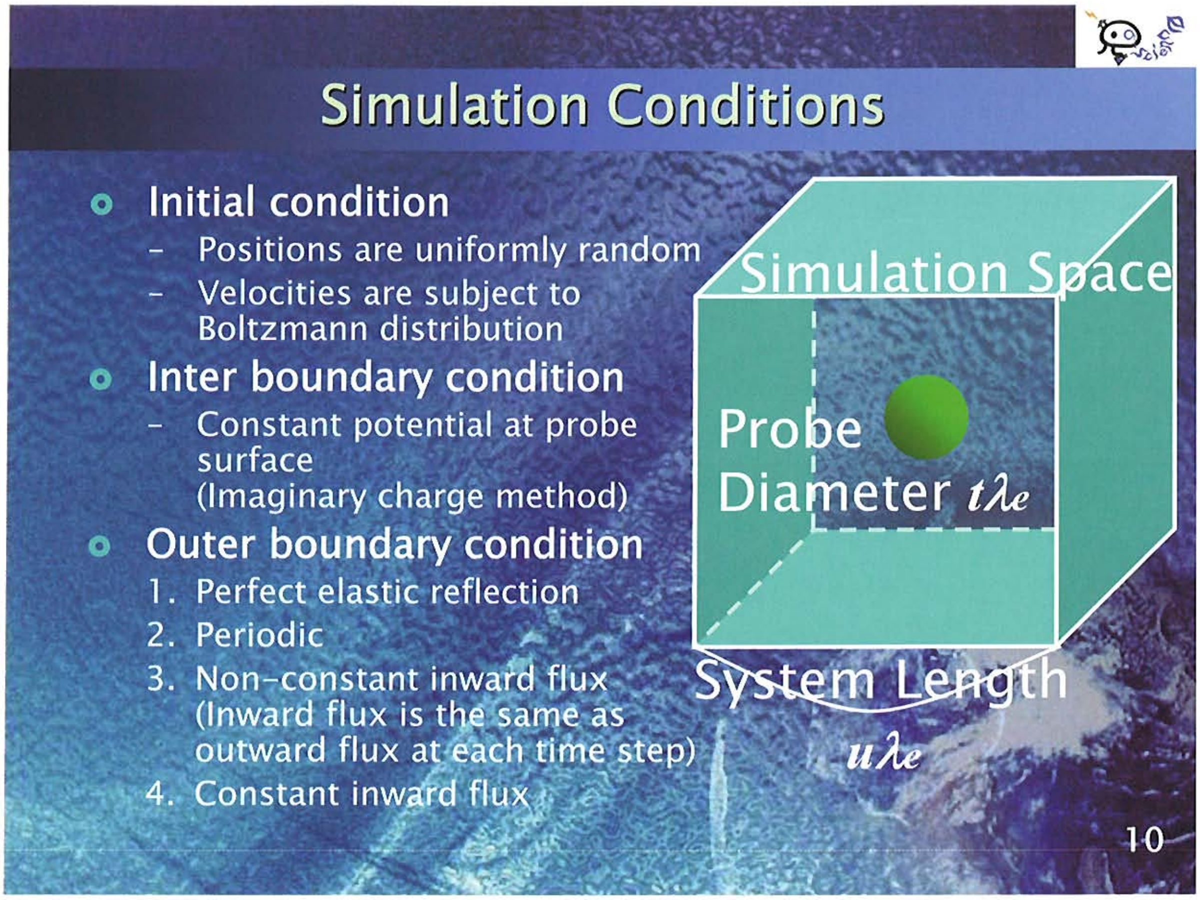
Simulation Conditions
Initial condition
- Positions are uniformly random
- Velocities are subject to Boltzmann distribution
Inter boundary condition
- Constant potential at probe surface (Imaginary charge method)
Outer boundary condition
1. Perfect elastic reflection
2. Periodic
3. Non-constant inward flux (Inward flux is the same as outward flux at each time step)
4. Constant inward flux
Simulation Space
Probe
Diameter $t\lambda_e$
System Length
$u\lambda_e$
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## Time Evolution

- Coulomb force is calculated by GRAPE-6

$$\phi_i = \frac{1}{4\pi\varepsilon_0}\sum_{j\neq i}\frac{q_j}{\left(r_{ij}{}^2+\varepsilon^2\right)^{1/2}}$$

$$\boldsymbol{a_i} = \frac{q_i}{m_i}\nabla\phi_i = \frac{1}{4\pi\varepsilon_0}\frac{q_i}{m_i}\sum_{j\neq i}\frac{q_j}{\left(r_{ij}{}^2+\varepsilon^2\right)^{3/2}}\boldsymbol{r_{ij}}$$

- Time integration is calculated by host MPU (Leapfrog method)

$$\boldsymbol{r}(t+\Delta t) = \boldsymbol{r}(t)+\boldsymbol{v}(t)\Delta t+\frac{1}{2}\boldsymbol{a}(t)\Delta t^2$$

$$\boldsymbol{v}(t+\Delta t) = \boldsymbol{v}(t)+\frac{1}{2}\left[\boldsymbol{a}(t)+\boldsymbol{a}(t+\Delta t)\right]\Delta t$$

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## Time Interval Limitation

- Limitation by thermal velocity

$$\sqrt{\left\langle v_{ex}{}^2\right\rangle}\Delta t = s\lambda_e\,(0<s<1) \Rightarrow \Delta t = s\left(\frac{\varepsilon_0 m_e}{e^2 N_e}\right)^{1/2}$$

  - In this work, s is chosen as

$$s = \frac{1}{128}$$

※The same result also comes from the limitation by plasma frequency

$$\omega_e\Delta t = s\,(0<s<1) \Rightarrow \Delta t = s\left(\frac{\varepsilon_0 m_e}{e^2 N_e}\right)^{1/2}$$

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## Particle Number Limitation (1)

- Limitation by memory cost
  - Position, velocity or acceleration costs each 24 bytes
  - Maximum memory is about 1GB on a single workstation

$$N \le 10^7$$

- Limitation by calculation cost
  - This is most dominant factor in a particle method
  - A few hundred time step can be calculated in a day on a single workstation hosting GRAPE-6 board
  - One time step is about 30 sec when N=262,144 and using O(N^2) direct scheme with GRAPE-6 board

$$N \le 10^6$$

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## Particle Number Limitation (2)

- Limitation by electron current resolution
  - Current induced by a single electron is much smaller than the theoretical current in Langmuir probe whose potential is zero

$$i_e = \frac{e}{\Delta t} = \frac{e}{s\lambda_e}\sqrt{\left\langle v_{ex}{}^2 \right\rangle} = \frac{e}{s\lambda_e}\left(\frac{k_B T_e}{m_e}\right)^{1/2}$$

$$I_{e0} = \frac{1}{4} e N_e S \langle v_e \rangle = \frac{1}{4} e N_e \pi (t\lambda_e)^2 \left(\frac{8 k_B T_e}{\pi m_e}\right)^{1/2}$$

$$\frac{i_e}{I_{e0}} = \sqrt{\frac{2}{\pi}} \cdot \frac{1}{s t^2 \lambda_e{}^3 N_e} = \sqrt{\frac{2}{\pi}} \cdot \frac{1}{s t^2 N_{eD}} \quad \left(N_{eD} = \lambda_e{}^3 N_e\right)$$

$$\frac{i_e}{I_{e0}} < \frac{1}{10},\ s = \frac{1}{128},\ t = \frac{1}{4} \Rightarrow N_{eD} > 1.63 \times 10^4$$

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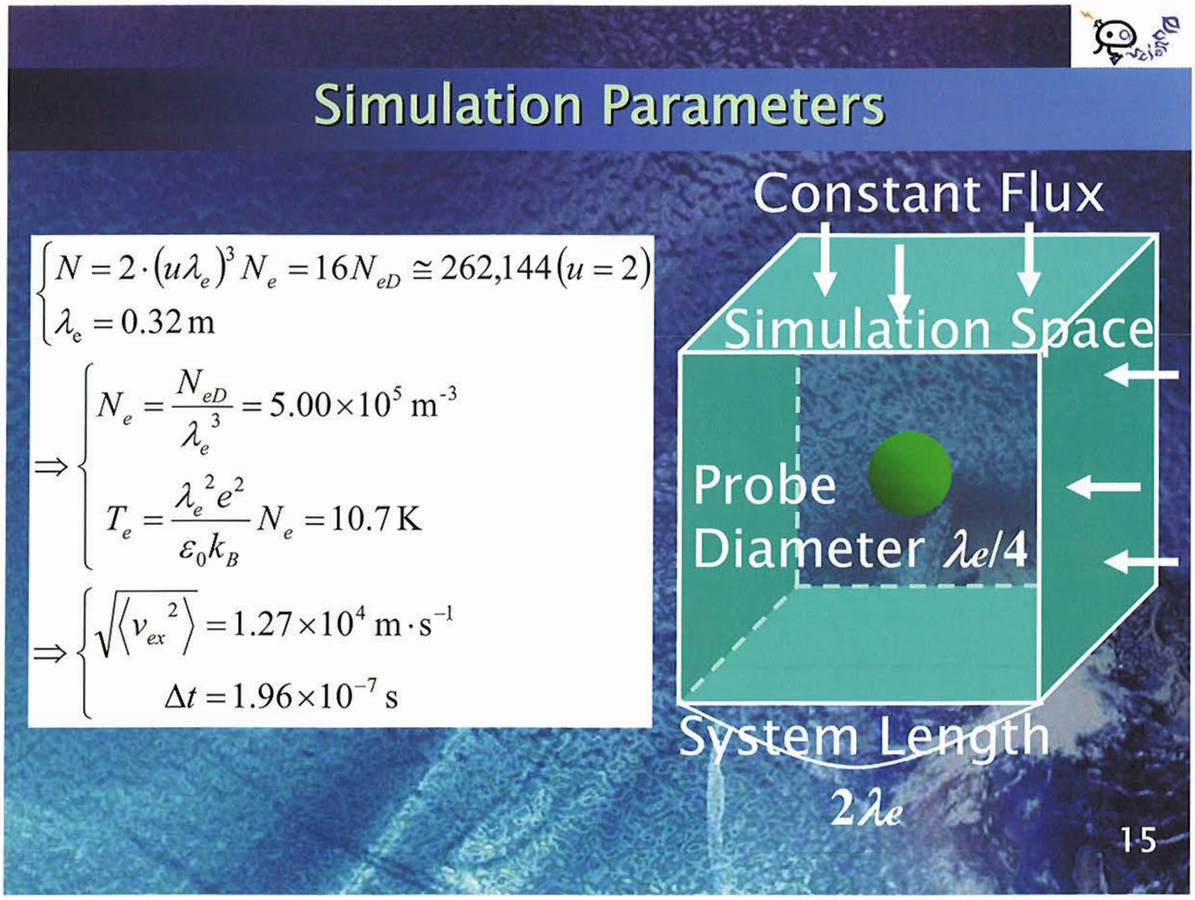
Simulation Parameters
$N = 2\cdot(u\lambda_e)^3 N_e = 16N_{eD} \cong 262{,}144\,(u=2)$
$\lambda_e = 0.32\,\mathrm{m}$
$\Rightarrow N_e = \frac{N_{eD}}{\lambda_e^{\ 3}} = 5.00\times10^5\,\mathrm{m}^{-3}$
$T_e = \frac{\lambda_e^{\ 2}e^2}{\varepsilon_0 k_B} N_e = 10.7\,\mathrm{K}$
$\Rightarrow \sqrt{\langle v_{ex}^{\ 2}\rangle} = 1.27\times10^4\,\mathrm{m\cdot s^{-1}}$
$\Delta t = 1.96\times10^{-7}\,\mathrm{s}$
Constant Flux
Simulation Space
Probe
Diameter $\lambda_e/4$
System Length
$2\lambda_e$
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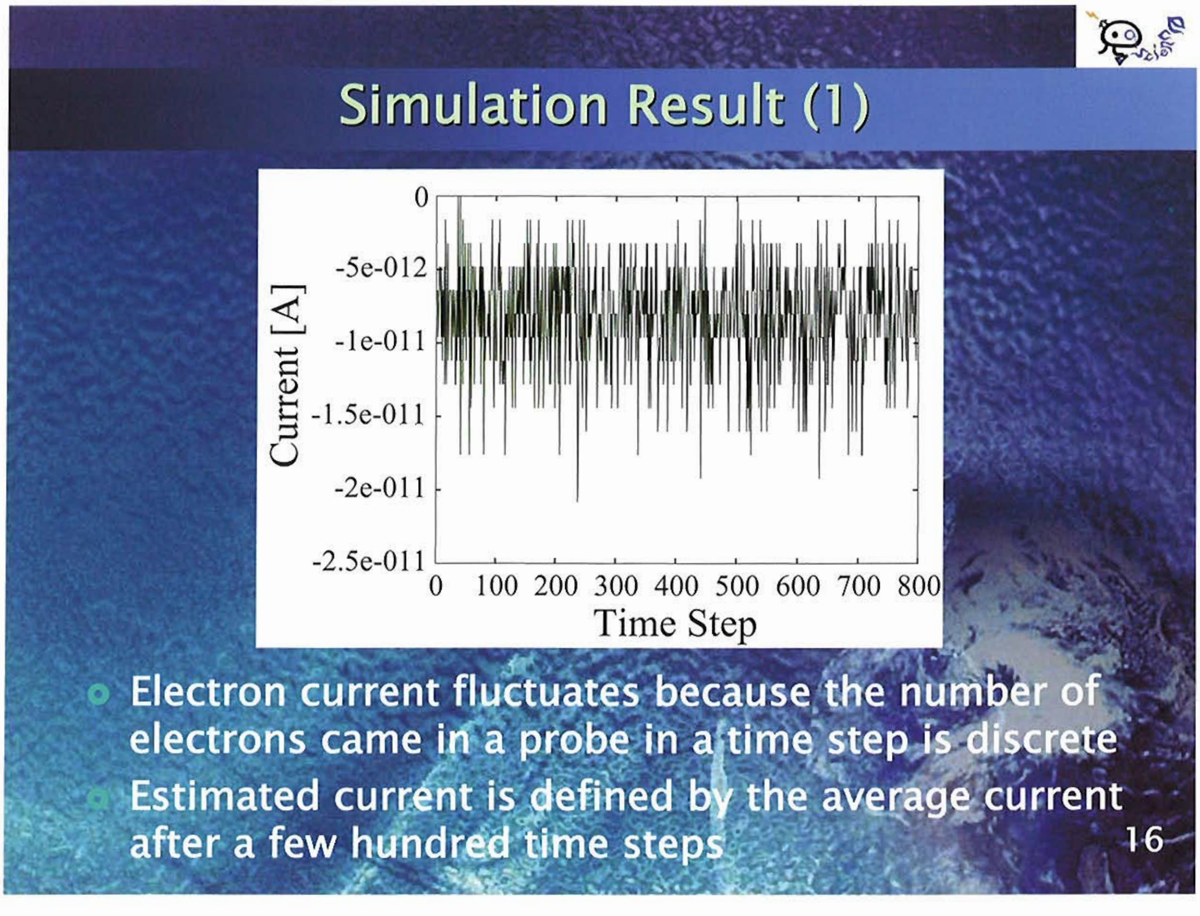
Simulation Result (1)
Current [A]
0
-5e-012
-1e-011
-1.5e-011
-2e-011
-2.5e-011
Time Step
0 100 200 300 400 500 600 700 800
Electron current fluctuates because the number of electrons came in a probe in a time step is discrete
Estimated current is defined by the average current after a few hundred time steps
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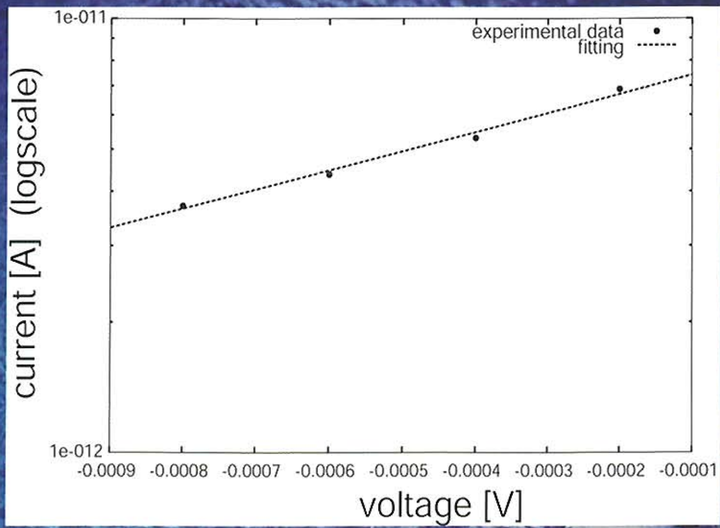
## Simulation Result (2)

- Estimated Ne and Te from Langmuir probe I-V characteristic (right figure)




| | Simulation | Theory | Error |
|---|---|---|---|
| Ne | 4.99e5 | 5.00e5 | 0.24 % |
| Te | 11.4 | 10.7 | 6.5 % |

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## Conclusion

- Micro-scale plasma simulation with O(N^2) direct scheme is performed on a single workstation with GRAPE-6
  - Calculation time with GRAPE-6 is 14 hours (400 time steps) while without GRAPE-6 it is about 1 month
- Assumed and estimated value of Ne and Te is very close in the negative low voltage limit
  - It is probable error is enlarged in the negative high voltage limit because ie/Ie becomes large
  - ie/Ie0=1/10 is not enough small

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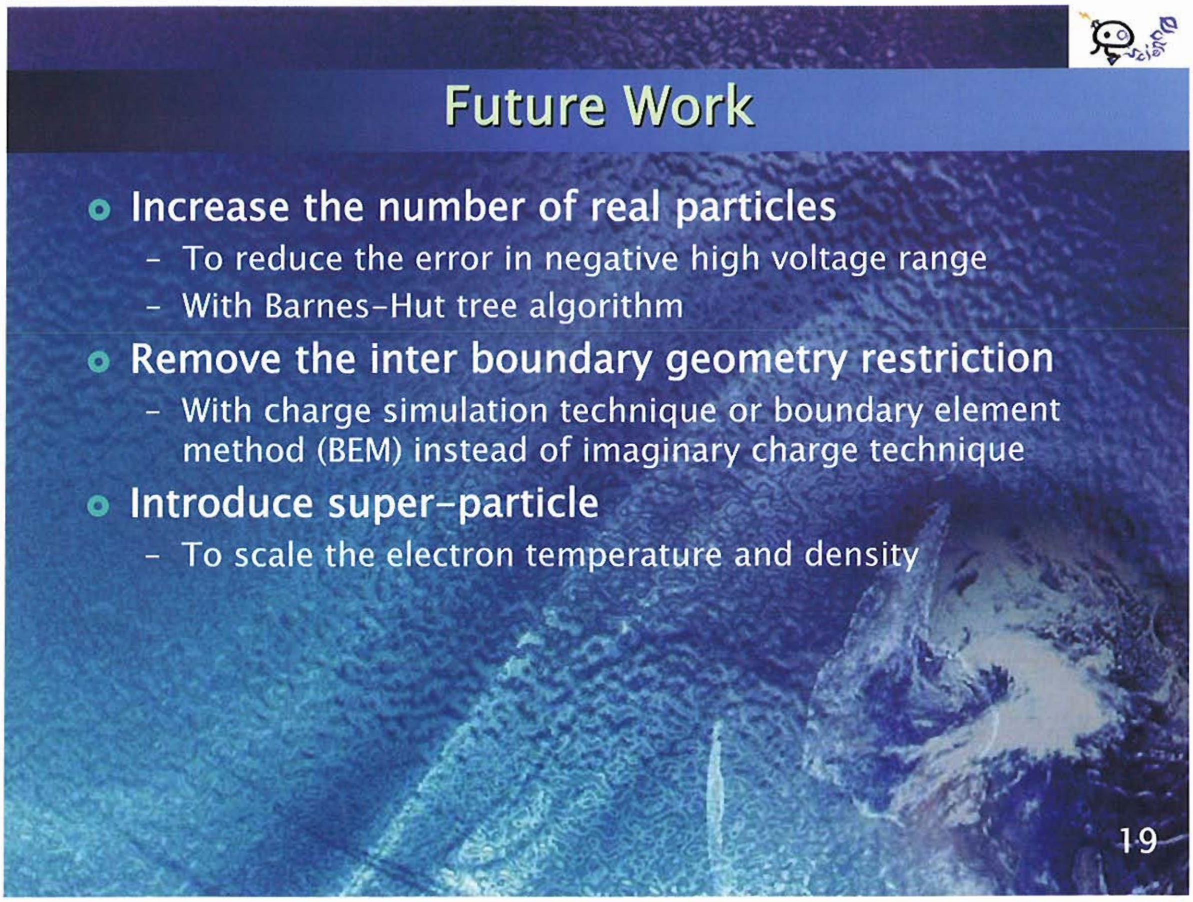
Future Work
Increase the number of real particles
- To reduce the error in negative high voltage range
- With Barnes-Hut tree algorithm
Remove the inter boundary geometry restriction
- With charge simulation technique or boundary element method (BEM) instead of imaginary charge technique
Introduce super-particle
- To scale the electron temperature and density
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