Large-scale Simulation for a Tera Hz Resonance Superconductors Device

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We are proposing a large-scale simulation of a Josephson-coupled superconductors (intrinsic Josephson junctions: IJJ) device which has a potential of Tera Herz resonance phenomena. This simulation should deal with nonlinear and complex systems and would require high performance computational resource. This is because a scale of space and time for simulation is 1nm-100 μm and 10^7 steps by 1fs. It is estimated that the calculation for simulation could take ten years to perform this simulation for only one case by a conventional computer. The Earth Simulator is therefore essentially needed for solving this problem through simulations. We show our recent result of Tera Hz resonance superconductors device simulation on Earth Simulator.

Keywords: intrinsic Josephson junctions, Tera Herz resonance, high performance computational resource

1. Introduction

The unexpected plasma phenomenon with the low frequency in the crystal of the high temperature superconductors whit connected multi layers (IJJ), was found by professor Uchida of The University of Tokyo in 1992. IJJ is formed in a single high temperature superconductors crystals of CuO_2 and insulator layers which form a stack of many atomic-scale Josephson junctions. IJJ has two kinds of Josephson plasma, one is the longitudinal plasma vertical to layers(c axis direction), another is the transverse plasma along layers (ab plane).

Afterwards, professor Tachiki of Tohoku University systematized the new phenomenon in the theory, and showed that the plasma oscillation wtih Tera Herz class is theoretically possible [1], [2]. In addition, the electromagnetic wave absorption of the plasma oscillation of IJJ was observed by professor Matsuda of University of Tokyo.

IJJ has a potential for an important industrial infrastructure technology in next generation; the super-high-speed computer, the storage elements, and high-capacity and high-speed optical communication conversion devices in the highly-networked information society. Leading countries scurry to develop this technology now. Japan is now leading still on both sides of the experiment and the theory research.

If we practiced at first the use in the world, it brings a large advantage to Japan in the area of a high-speed computer and the information on telecommunications equipment, etc. and has the possibility to throw up the Japanese original new industry as a strategic technology in Japan. In semiconductor area of a basic research advanced by the United States, Japan was under an accusation with the free ride of a basic research. But, our country does not cause international friction in the IJJ technology area because this technology is developed from a basic research in Japan.

IBM had developed a high speed switch consisting of the lead single-junction Josephson device in 1980's. That Josephson device broke down in one month from one week and practical use was impossible. Fujitsu and Electrotechnical Laboratory had tried to develop the niobium single-junction Josephson high speed switch. That development was discontinued due to mismatching between the semi-conductor memory and Josephson device.

In contrast, the target by this challenge using IJJ is a new device which differs from past Josephson devices. It is tough because of consisting of monocrystalline, and it is possible to use almost permanently. Since IJJ device has a special character, a generation of the Tera Herz electromagnetic wave will be possible.

IJJ device is utilized as the next generation device such as the Tera Herz electromagnetic wave generator. If this would achieved, it is possible to develop the large capacity and super-high-speed next-generation computer which is higher speed of three order of magnitude and three order low power consumption compared with a present high-speed computer. It is expected that the optical transmission capacity and speed improve explosively, and the large capacity high-speed information communication is realized by Tera Herz electromagnetic wave.

The development of the Tera Helz electromagnetic wave generation is a very dicult only by the experiment, because IJJ have a very strong nonlinearity and the complex behavior. The development research on the simulation base is indispensable. However, this simulation should deal with nonlinear and complex systems and require high performance computational resource. This is because a scale of space and time for simulation is 1nm-100 μm and 10^7 steps by 1fs. It is estimated that the calculation for simulation could take ten year to perform this simulation for only one case by a conventional computer. The Earth Simulator is therefore essentially needed for solving this problem through simulations. So to speak, it can be said that only the earth simulator will enable the next generation super-high-speed computer to develop. We have tuned the simulation code for Earth Simulator, and got some results. Let us to show our simulation method and results.

2. Model Equation

The physical system which should be solved the equation of system consists of IJJ and the external medium.

In IJJ, a coupling equation of the gauge-invariant phase difference φ_k, charge ρ and electric field E^z, which is derived from Josephson relation and Maxwell equation, is solved. The gauge-invariant phase difference is a phase difference between superconducting layer l+1 and l layer .

It is related to Josephson's superconducting electric current. Maxwell equation is solved at the outside of IJJ. Let us show a formulation for analysis model. The equations describing the dynamics of the phase difference, charge and electric field are given by

$$\left(1-\frac{\lambda_{ab}^2}{sD}\Delta^{(2)}\right)\Big[\frac{\partial^2\varphi_k}{\partial t'^2}+\beta\frac{\partial\varphi_k}{\partial t'}+\sin(\varphi_k)+\frac{\varepsilon\mu^2}{sD}\left(\Delta^{(1)}\frac{\partial\rho'_k}{\partial t'}+\beta\Delta^{(1)}\rho'_k\right)\Big]=\frac{\partial^2\varphi_k}{\partial x'^2} \quad (1)$$

$$\left(1-\frac{\varepsilon\mu^2}{sD}\Delta^{(2)}\right)\rho'_{k+1/2}=\frac{\lambda_c}{s}\Delta^{(1)}\frac{\partial\varphi_{k+1/2}}{\partial t'} \quad (2)$$

$$\left(1-\frac{\varepsilon\mu^2}{sD}\Delta^{(2)}\right)E'^z_k=\frac{\partial\varphi_k}{\partial t'}. \quad (3)$$

At outside of IJJ, Maxwell equation is as follws,

$$\frac{\partial E'}{\partial t'}=\nabla\times B'-J' \quad (4)$$

$$\frac{\partial B'}{\partial t'}=-\nabla\times E'. \quad (5)$$

where $\Delta^{(2)}A_k$ *is* $A_{k+1}-2A_k+A_{k-1}$, k : number of insulator layer between uperconducting layer l and l+1, σ: conductivity of the quasiparticles, ε : dielectric constant of the insulating layers, μ: the Debye lenght, Φ_0 : unit magnetic state, J_c : critical current density, s, D : superconducting and insulating layer thikness, φ_k : gauge-invariant phase difference in insulator layer k, $\rho_{k+1/2}$: charge density in superconducting layer in k+1/2, E_k^z : electric field in z direction at insulator layer k, λ_{ab} : penetration depth in the ab-plane direction,

$\lambda_c=\sqrt{\frac{c\Phi_0}{8\pi^2 DJ_c}}$: penetration depth in the c axis direction,

$\beta=\frac{4\pi\sigma\lambda_c}{\sqrt{\varepsilon}c}$, $\omega_p=\frac{c}{\sqrt{\varepsilon}\lambda_c}$: Josephson plasma frequency,

$t'=\omega_p t$: normalized time, $x'=x/\lambda_c$: normalized coordinate in x direction, $\rho'=\rho/(J_c/\lambda_c\omega_p)$: normalized charge density, $E'^z=E^z/(2\pi cD/\Phi_0\omega_p)$: normalized electoric field in IJJ, $\boldsymbol{E}'=\boldsymbol{E}/(2\pi cD/\Phi_0\omega_p)$: normalized electoric field, $\boldsymbol{B}'=\boldsymbol{B}/(2\Phi_0\omega_p/cD)$: normalized magnetic field.

These equations are solved by Finite Difference Method. Some research [3] has been done based on this model.

3. Computational Feature of IJJ Simulation

IJJ phenomenon is very strong nonlinear and complex. Many researchers try to understand IJJ phenomenon via experiments and analytical methods. But, it is very hard to understand IJJ phenomenon with only experiments and analytical method. IJJ simulation based on the model equation can show a detail of IJJ phenomenon mechanism, can allow researchers to easily change a conditions of numerical experiments to evaluate the effect of many conditions. Therefore, IIJ simulation opens up great possibilities for a development of IJJ technology.

It is estimated that the calculation for simulation could take ten years to perform this simulation for only one case by a conventional computer. This is because a scale of space and time for simulation is 1nm-100 μm and 10^7 steps by 1fs. In addition, many times IJJ simulation which are with combination of many different material properties, device shapes, current supply methods and current control etc is needed to design and optimize the Tera Hz resonance superconductors device. Therefore, IJJ simulation requires high performance computational resource.

4. Parallel Vector Tuning and Performance

The simulation program exploring mainly the transverse plasma wave emission is constructed by two solvers for the coupled sine-Gordon and the Maxwell equation. The computational region is an one-dimensional junction array composed of several intrinsic Josephson junctions aligned on a substrate. We solve the coupled sine-Gordon equaiton for intrinsic Josephson junctions and the Maxwell equation in the cavity regions between intrinsic Josephson junctions. Now, let us show results for performance tests of the program on Earth Simulator. The vector operation ratio of the code is 99.6% the oating operation counts per sec (Flops) for any cases exceeds over 4.0Gfops in 1PE execution without no parallelization. This result indicates that vector performance is always beyond a half of the peak performance. This is because the coupled sine-Gordon equation shows very high operation density since it has many terms with high oating operations, e.g., there are terms including calculations of sin function. This character is quite favorable for the vector supercomputer. On the other hand, the parallelization ratio is above 99.9%. In all simulations, a sub-set region composed of a few intrinsic Josephson junctions and neighbor cavities is allocated for 1 processor, and hundreds or thousands of the subsets are simulated by using several nodes on Earth Simulator. Then, the overlapped regions between the sub-sets are communicated between virtually neighboring processors, but almost communication times are hidden by the calculations. The reason is that the overlapped region required for the Maxwell equation is communicated during the calculation of the sine-Gordon equation, and vice versa. These results show that the code is quite effective for massively parallel type of supercomputer like Earth Simulator. Thus, we believe that this simulation code may be one of the most effective code on Earth Simulator.

5. Simulation Models and Results

(1) Antenna Radiation Model with Longitudinal Plasma

The device based on Josephson Vortex resonating with transverse plasma will have very strong radiation power. That is very useful for height power main generator of Tera Hz wave. But this device requires an external applied magnetic field generator.

If the Tera Hz radiation could be possible without external magnetic field, the Tera Hz resonance superconductors device could have simpler and became small size. That is very important for micro-electronics applications. The device based on antenna radiation model have a very simple structure which is showed in Fig. 1.

If AC Josephson effect generates the displacement current which have a very large magnitude and if the displacement current radiates from the top and bottom surface vertical to c axis of IJJ, IJJ would work as antenna. The radiated displacement current could generate electromagnetic waves at an outside of IJJ. A cavity which has a large dielectric constant would absorb the electromagnetic waves, would enhance a power of the electromagnetic waves and would radiate Tera Hz strong electromagnetic waves.

The antenna model simulation used olny the equations Eq.

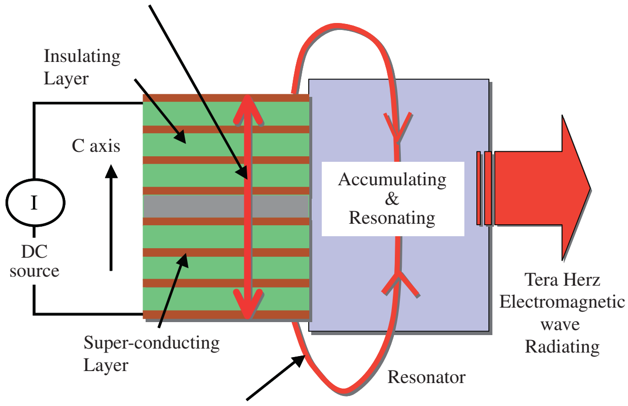

Fig. 1 Schematic diagram of antenna radiation model.

(1), Eq. (2) and Eq. (3) at this time. At the boundary in the ab-plane direction, the boundary condition is written as Eq. (6), where $\acute{B}^{y}_{k0}$ is the current induced magnetic field correspond to the left and right edge. In the c axis direction, the boundary condition is written as Eq. (7). bottom of IJJ. The γ means a radiation ratio of displacement current.

$$\frac{\partial \varphi_k}{\partial x'} = \acute{B}^{y}_{k0} \tag{6}$$

$$\acute{\rho}_{k\pm 1/2} = \gamma \frac{\lambda_c}{s} E'_k \tag{7}$$

$$\frac{\partial \rho'_{k\pm 1/2}}{\partial t'} = \gamma \frac{\lambda_c}{s} \frac{\partial E'_k}{\partial t'} \tag{8}$$

We have got a results which shows that there are coherent displacement current with large amplitude by 1D, 2D small models. The number of junctions in real IJJ is from 1,000 to 10,000, very large number. It was expected that behavior between small number and large number junctions is different because intrinsic Josephson junctions has very strong nonlinearity. The result of three preliminary models are showed at here. Width is 0.1μm to parallel ab-plane (10 cells) and number of junctions is 20, 50, 100 (0.03, 0.075, 0.15μm) to c axis. Fig. 2 shows the results. This results show that a displacement current in IJJ increase rapidly corresponding to increasing of numbers of junctions. This means there are possibility that the large number of junctions IJJ could generate a very strong electromagnetic waves. We would like to study this possibility using Earth Simulator.

(2) Radiation Model based on Josephson Vortex Resonating with Transverse Plasma

We confirme that the ultra large-scale simulation is straightforward and is very useful for understanding real device arrangements. In this section, we show a preliminary result instead of our nal ones. But, it rides on a line of our target. Fig. 3 (a) is a part of characteristic I-V curve obtained in numerical simulations for the one-dimensional junction

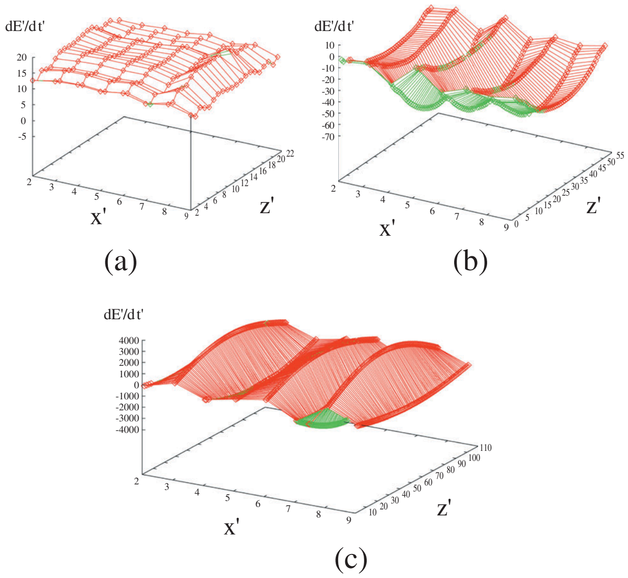

Fig. 2 Displacement current in IJJ by preliminary models simulation. t'=3.5, x' axis: parallel to ab-plane, z' axis: parallel to c axis, $\frac{dE'}{dt'}$: displacement current to z' axis, β=0.03, α=0.1, γ=0.1, the external constant current I'=1.04 in this simulation. (a) 20 junction (b) 50 junctions (c)100 junctions.

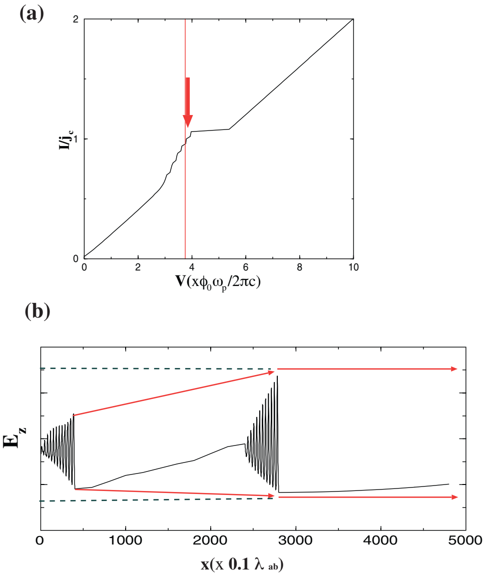

Fig. 3 (a)The I-V characteristics for the system of the junction array embedded inside a wave guide.(b) The snapshot of the spatial distribution of the electric field excited in the system.

array model composed of several intrinsic Josephson junctions. The I-V curve shows a nonlinear resonant behavior at the middle of the figure. The red line indicates the most nonlinearly amplified voltage-point. Then, the electric field distribution inside the junction array is given by Fig. 3 (b), where the electric field varies rapidly and slowly the inside intrinsic Joseph-son junction and the cavity, respectively. From the figure, it is found that two junction areas interact via the electro-magnetic wave propagation in the cavity region and the electric field is amplified along the uni-axial direciton (x-direction). This is because the transvers plasma is excited inside the junction area from the left to the right hand side and connected into the cavity region as the electro-magnetic wave. Moreover, we find that the electric field in the right hand side of junction area is more enhanced. This result clearly shows that two neighboring junctions resonate and emit stronger electromagnetic wave than the single junction. In the future work, we will investigate this type of amplification process due to resonances between hundreds or thousands of intrinsic Josephson junctions by using Earth Simultor. Up to now, we have succeeded to simulate an array of 4096 intrinsic Josephson junctions as a test problem. In the next pyscal year, our task will be a challenge to unknown nonlinear resonant-amplification problems in ultra large-scale.

6. Future Work

In this year, we have mainly concentrated on checking the performance of the simulation code on Earth Simultor for this subject as shown above. Therefore, we have not yet acheived final results, but clarified that the code performance is quite high.

A design condition for Tera Hz resonance superconductors device based on the antenna radiation model and radiation model based on Josephson vortex resonating with transverse plasma will be studied on Earth Simulator.

7. Conclusion

We have got the good performance of program for Tera Hz resonance superconductors device simulation. We believe that Earth simulator class or over class high performance computational resource only enable us to research and design for Tera Hz resonance superconductors devices.

References

[1] M.Tachiki, T.Koyama, and S.Takahashi, Electromagnetic phenomena related to a low frequancy plasma in cuprate superconductors, Phys. Rev. B 10, 7065, 1994.

[2] M.Tachiki, T.Koyama, and S.Takahashi, in: G.Deutcher, A. Revcolevshi(Eds.), Coherent I High Temperature Superconductors, World Scientific, Singapore, 1996, p.371.

[3] M.Tachiki, and Masahiko Machida, Current Understanding of Josephson Plasma Theory and Experiments in HTSC, Physica C 341-348(2000) 1493-1498.

テラヘルツ発振超伝導素子に関する大規模シミュレーション

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1. 具体的な研究目的

酸化物高温超伝導体はそれ自体がジョセフソン結合系を形成しており、テラヘルツに振動数領域をもつジョセフソン・プラズマというシャープな励起状態が存在する。定電流・定電圧をかけたとき起こる交流ジョセフソン周波数と共鳴したとき強い発振が起こることが期待される。テラヘルツ発振のみならず、光通信の情報量の増大、ひいては超高速、低電力計算機を製作することが可能である。これら素子の設計には地球シミュレータの使用が必須である。以上のような可能性を背景に、本研究では、テラヘルツ発振超伝導素子に関する大規模シミュレーションの研究を目的とした。

2. プログラムの簡潔な説明

- 解くべき物理系・基礎式：ジョセフソン素子内とその外部媒体からなる。
  - ・ジョセフソン素子内部：量子論的な不変ゲージ位相の式を時間・空間で微分したジョセフソンの関係式とマックスウエル方程式から得られる、ゲージ不変位相の式と電荷の式を連立した式。サイン・ゴルドン方程式のサイン項、ゲージ不変位相の時間微分項が、拡散型の階差式で連成した極めて非線形性の強い式。
  - ・素子外部の媒体部：不均質媒体中のマックスウエル方程式。
  - ・2つの領域の接続：マックスウエルの方程式とジョセフソン結合の超伝導の基礎方程式を組み合わせた接続方程式。
- 計算規模：例えば、1層1nmの厚で、全体で100μm程の寸法となるテラヘルツ発振する固有ジョセフソン結合素子をシミュレーションするためには、通常のPCでは、1ケース10年もかかってしまう。しかも多種類のモデルによる多数回のシミュレーションにより最適な素子を見つけなければならない。

3. 地球シミュレータを利用してこれまでに得られた今年度成果

- 大規模高速計算チューニング：並列化率 99.9%、ベクトル化率99.6%（10^7～10^8セル）
- 大規模シミュレーションでの解の挙動の大まかな把握：縦プラズマアンテナ発振、横プラズマ励起発振両モデルにて、予備的解析を行い、物理的にも有用な知見が得られつつある。

4. 来年度以降の計画

- 来年度は、今年度の結果に基づく解析コード（解析アルゴリズム、結合素子境界接合法等）の改造、再度のチューニング、テラヘルツ発信条件発見のための多数回の探索計算を行う。
- 16年度の研究内容は、14、15年度の成果により決定する。

キーワード：固有ジョセフソン結合素子、テラヘルツ発振、大規模高速計算資源