Large-scale Parallel Fluid Simulations for Spallation Type Mercury Target Adopted in the Project of High-intensity Proton Accelerator

Group Representative
Chuichi Arakawa Center for Promotion of Computational Science and Engineering, Japan Atomic Energy Research Institute, Group Leader

Authors
Chuichi Arakawa Center for Promotion of Computational Science and Engineering, Japan Atomic Energy Research Institute, Group Leader
Norikazu Goto Center for Promotion of Computational Science and Engineering, Japan Atomic Energy Research Institute

The mercury target works as a high-density neutron source by the nuclear spallation reaction resulting from the hitting of mercury atoms with highly accelerated protons. In the spallation reaction process, high-density heat is released simultaneously and generates shock wave in mercury. One difficulty in applying this spallation reaction is the release of higt-density heat which result in the generation and propagation of shock waves through the liquid mercury. The aim of this project is to determine the most optimized design of the Mercury target. In order to achieve the objective by numerical simulations, models with very fine meshes are required. Such type of simulations heavily requires computational resources, i.e. fast processing elements and large amount of memory storage.

Our initial target for the latter half of year 2002 is to refine our thermal-hydraulic calculation code to run on sufficient number of nodes. In the preliminary calculation, small- scale model is considered and the ratios acquired for vectorization and parallelization were 99.6% and 100% respectively. We believe these numbers are promising. On the other hand, we found that bank conflicts occur in one of the most time-consuming routine. We are currently making farther developments to reduce the number of bank conflicts.

keywords: Mercury target, thermal-hydraulic calculation

Report of Results

Project Outline

This project focuses on Mercury target used for neutron sources in high-density neutron scattering laboratory constructed as a plan of the high-power proton accelerator project. The structure of the Mercury target is a pipe like channel made by SU316 as depicted in Fig.1, and liquid Mercury circulates inside the channel. The protons come from the perpendicular direction to the flow channel and collide with the target. Then, Mercury emits neutrons due to the nuclear fission caused by the collisions with protons. High -density energy releases by the nuclear fission cause strong shock waves inside the Mercury target. Thus, the fact gives a limitation on the construction plan for the outer wall of the pipe channel. Furthermore, recent experiments in the shock wave reflection at the liquid-solid interface revealed that the outer wall suffers fine damages due to cavitations created after the deep impact by the shock waves into the wall. Thus, the construction plan of the Mercury target should consider not only the simple shock wave pressure but also the cavity damage. Our final target is, therefore, to conduct the future construction plan by performing precise numerical simulations involving the cavity nucleation and explosion processes. This is a quite challenging task but has a great impact on wide engineering fields if the simulation is successful.

Simulation Program

The simulation program adopts the finite volume method in order to simulate dynamics of compressible thermal fluids. The mercury target geometry is discretized by a regular grid with 3-dimensional generalized coordinate. We can select a proper boundary condition for the inlet boundary among the fixed and the free boundary conditions, and similarly, for the wall boundary among the slip and non-slip boundary conditions. The advective term is differenciated by the first-order upwinding scheme or the central difference. The time integration is carried out by the HSMAC scheme and the BiCGSTAB iterative solver was implemented for

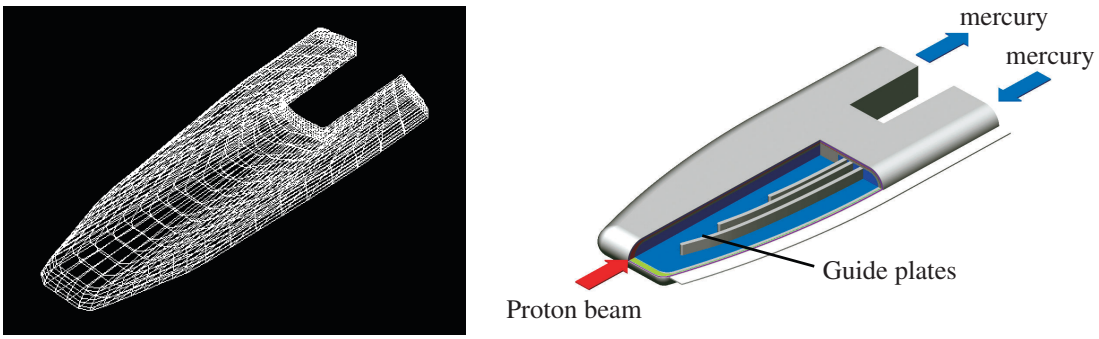

Fig. 1 Mercury target over view

solving the Poisson's equation. The complete set of equations are composed of the mass, the kinetic momentum, and the energy conservation equations with the state equation for liquid Mercury. This set enable us to simulate liquid Mercury dynamics inside the Mercury target.

Vectorization and Parallelization

Our parallelization strategy is basically a spatial decomposition, in which each processor has its own calculation region and communicates with other processors only when it needs informations outside the region. These procedures are all described by standard MPI. In excutions, MPI communications occur in steps of the advective term calculation and the iteration by Bi-CGSTAB. In the former step, a difference in the boundary requires neighboring processor's regions, while the total product calculations in the latter step request all processor's communications. For I-O, this code is also parallelized. The initial data is pre-divided to smoothly follow parallel calculations and the output is parallelized similarly. Thus, all processesings including I-O are executed under the same parallelization strategy. The vecotorization is also implemented and the vector lengths are taken as long as possible for large data. We performed test simulations about a million grid points on the Earth Simulator. As a result, we obtained satisfactory performances, i.e., the average of the vectorization ratio is 99.6% and the parallelization effect is maximum 100%. In order to check the parallelization effects, we compared a test case whose mesh size is 800x500x30 by using 32CPU and 64 CPU. In 32 and 64 CPU cases, the computational region is, respectively, divided into 8x4x1 and 8x8x1 blocks to keep the cell size inside each block equally. We show the vectorization and the parallelization effects in more detail in the following.

The vectorization effects

We believe that the vectorization is fully achieved. The vectorization ratio exceeds over 99.7% in a routine whose computation time accounts for about 90% of the total time. Furthermore, even in the total computation including I-O routines it shows 99.6%.

The parallelization effects

The test calculations using 32 and 64 CPU take 3259 and 1563 sec, respectively. This result indicates that the parallelization ratio exceeds over 100% if we use a formula calculating the parallelization ratio from the comparison between two different CPU cases as given above. In other words, the 64 CPU case shows a better performance than the 32 CPU one although the communication counts in the 64 CPU is clearly larger. This is an unusual data in vector parallel type of supercomputers but a quite interesting one since the mechanism may be related with an essential problem in parallelizing the iterative calculation algorithm using Bi-CGSTAB method. We now examine whether or not the reason is connected with a difference of the matrix created by the preconditioning. On the other hand, we found that bank conflicts occur inside a routine, which is ranked as a upper routine in computation counts. We are inspecting the reason because the routine is involved in the main algorithm itself.

Future works

Through test simulations on the Earth simulator in this year, we get a precise evaluation of the parallelization effect as our first goal. Further massive parallel calculations will make the problem to be improved clear. We can predict that almost computation time is mainly consumed by solving the matrix when the computation size increases further. Then, we expect to improve the total performance by implementing a matrix solver routine developed for the Earth simulator in our institute JAERI. Moreover, we will go toward improvements of modeling as a second our goal since modeling generally depends on the calculation precision, i.e., the direct simulation without any approximations may be accessible on the Earth simulator. In conclusion, the use of the Earth simulator enables us to open a possibility of fairly precise calculations. This inspires us to predict a limitation in the safety use of the Mercury target with fully reasonable simulation results.

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大強度陽子加速器計画で用いられる
核破砕水銀ターゲット内部の大規模並列流体シミュレーション

利用責任者
荒川　忠一　　日本原子力研究所　計算科学技術推進センター　並列計算法開発グループ　グループリーダー
著者
荒川　忠一　　日本原子力研究所　計算科学技術推進センター　並列計算法開発グループ　グループリーダー
後藤　記一　　日本原子力研究所　計算科学技術推進センター　並列計算法開発グループ

本課題は、大強度陽子加速器計画の一環として建設される高密度中性子散乱実験施設で中性子源として用いられる、核破砕タイプの水銀ターゲットに関するものである。水銀ターゲットは核破砕時に解放される多大な熱エネルギーとその結果生じる衝撃波に十分耐えるものでないといけない。更に、最近の実験では衝撃波が金属壁に微細な傷を発生させていることが分かり、衝撃波のあたう限り正確なシミュレーションの必要性が主張されている。そこで、圧縮性熱流体コードを大規模並列に実行することで、この問題を解決したいと考えている。

使用したコードは、地球シミュレータ用にチューニングを施した圧縮性熱流体解析コードで、有限体積法に基づくものである。時間積分にはHSMAC法を用い、BiCGSTAB法に基づく反復法で圧力のPoisson方程式を解いている。支配方程式は、質量保存・運動量保存・エネルギー保存・状態方程式である。状態方程式に水銀のものを採用することで、液体水銀の計算を行える。

このプログラムは計算領域を複数のブロックに分けて、各プロセッサに担当領域分の計算を分配する方法で並列化を計っている。また、各プロセッサは担当領域のみの物理量をメモリに保持し、計算過程で領域外の物理量が必要になった場合にはMPIを用いて値を入手する。このプログラムは、計算用初期データとしてあらかじめ領域ごとに分割して製作したものを読み込む様になっており、データの入出力まで含めパラレルに処理が進むように工夫されている。また計算ループのうち大きな物は1次元化が施してあり、ベクトル長が十分な長さになるようになっている。

このプログラムで、約1千万格子点のモデルに対して計算を実行してベクトル化率・並列化率を計算してみた。比較は32並列計算と64並列計算で行った。その結果、ベクトル化率は両計算とも、計算時間の9割を占めるルーチンで99.7%を超え、入出力を含めた平均でも、99.6%を超えていた。また、両条件で30ステップずつ計算を行った結果、Real time は32並列では3259(s)、64並列では1563(s)を要し、この並列化効率から並列化率を算出すると100%となる。並列化率が100%を示した理由は今調査中であるが、このプログラムがBi-CGSTAB法に基づく反復計算を利用したものであり、前処理行列が分割数を変えた場合変化することに原因を求められるのではないかと考え、検証計算を続けている。

キーワード：水銀ターゲット、圧縮性熱流体