

Radial and Axial Domain Decomposition of a Core Thermal-Hydraulics Code for Massively Parallel Computing Platforms

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1. Introduction

Pin-resolved whole core multiphysics calculations become more practical through advanced computing resources and numerical methodologies. In particular, the subchannel-scale thermal-hydraulics (T/H) analyses are desirable for core multiphysics calculations because of their adequacy in terms of solution accuracy and computing time.

In that sense, Seoul National University initiated to develop a new core T/H code called ESCOT (Efficient Simulator of Core Thermal-Hydraulics) [1]. Even though state-of-the-art subchannel-scale T/H codes [2] are based on the two-fluid model, ESCOT adopted the four-equation drift-flux model (DFM) which has advantages of simple models for two-phase flows and cheap computational cost. The three-dimensional (3-D) domain of a reactor core is discretized by the Finite Volume Method (FVM) in a staggered grid system, and solutions are calculated by the Semi-Implicit Method for Pressure Linked Equation (SIMPLE)-like algorithm. The solution accuracy of ESCOT was validated through comparisons with experimental data and other subchannel-scale codes [3].

The ESCOT code aims at highly parallelized execution under a modern computing platform having multiprocessors and multiple machines. For that purpose, ESCOT is parallelized by employing radial and axial domain decomposition with the Message Passing Interface (MPI) library. In this paper, the features of parallelization of ESCOT is covered. The integrity of the parallel solutions will be demonstrated by the verification problems. Scalability analyses with conceptual problems and a OPR1000 quarter core problem are prepared to show the parallel performance of ESCOT.

2. Parallelization Scheme of ESCOT

2.1 Radial and Axial Domain Decomposition

Assembly or sub-assembly-wise radial domain decomposition can show a satisfactory parallel performance of a subchannel code [4]. Fig. 1 illustrates the assembly-wise radial domain decomposition applied for ESCOT.

Furthermore, the axial domain of ESCOT can be decomposed as many times as the number of axial planes. The radial-only decomposition forces the users to have a rigid and specific number of processors, which is one processor per assembly. The axial domain

decomposition can give users more flexible choice for the number of processors. In addition, thousands of processors are available for the parallel execution rather than a hundreds of processors through bidirectional (radial and axial) decomposition. For example, 177 processors will be assigned for an OPR1000 full-core model with the radial-only decomposition, but 354 processors or even 1,770 processors can be available with the bidirectional decomposition if users divide the axial domain into two or ten.

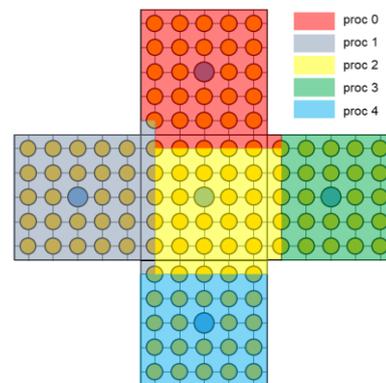


Fig. 1. Example of assembly-wise radial decomposition

ESCOT is parallelized by MPI to consider a distributed memory system, so the domain decomposition makes neighboring information at other subdomains unknown. Thus, one layer of ghost cells is allocated by surrounding a local subdomain, as Fig. 2 shows.

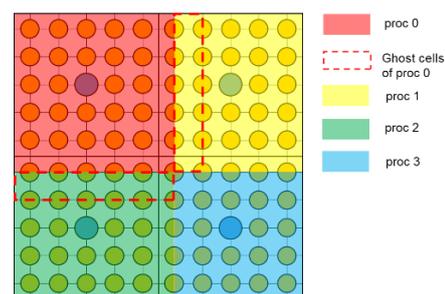


Fig. 2. Example of assigning ghost cells

2.2 Algorithm for Parallel Execution

The numerical solution scheme of ESCOT is the SIMPLEC (SIMPLE-Consistent) algorithm presented in Fig. 3. During an outer iteration, three main linear systems are solved: the axial momentum equation, the

lateral momentum equation, and the pressure correction equations. In particular, solving the linear system of the pressure correction equation is the most time-consuming part, so it is crucial to implement an efficient parallel linear solver. Hence, the Portable Extensible Toolkit for Scientific Computations (PETSc) [5] is linked to ESCOT, so that various Krylov Subspace Methods and preconditioners are easily employed in MPI parallelized platforms. Blue colored boxes in Fig. 3 denotes the points where the solver of PETSc library is used.

The ghost cells are received the updated solution of primary variables at every time level, so that the parallel solution is same as the serial solution. The points for neighboring data transferring via MPI communication are denoted by yellow boxes in Fig. 3. For the secondary variables, they can be updated locally through the steam table as the function of primary variables.

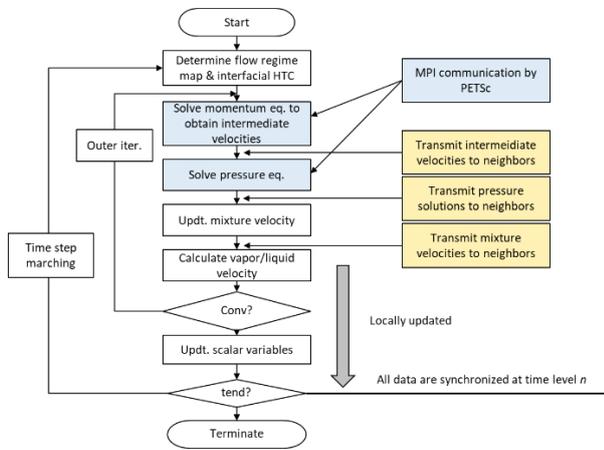


Fig. 3 Flowchart of SIMPLEC Algorithm of ESCOT with MPI data transferring points

3. Verification of Parallelization

In order to verify the parallel solution of ESCOT, two verification problems are constructed. Each problem consists of 16x16 rod bundles which represent typical fuel assemblies of Pressure Water Reactors (PWRs). The assemblies are arranged as shown in Fig. 4, and the five-assembly problem is included to consider the geometry types in full-core problems. The boundary conditions of Hot Full Power (HFP) of PWRs are given as 15.5 MPa outlet pressure, 3,501 kg/(m²·s) mass flux, and 16.5 MW power per assembly. The radial power profile is flat, while the axial power shape is a cosine shaped. The 3.81 m axial height is uniformly divided into 40 planes.

Theoretically, the parallel and serial solutions are identical. However, the very weak diagonal dominance of the pressure matrix leads to the unavoidable round-off errors when the order of the operations is switched [4], so solutions of two have few discrepancies. The relative errors of the parallel run are measured by subtracting the parallel solutions from the serial solutions and divided by the serial ones in SI unit. Fig. 5 shows the maximum

relative errors of mixture density, liquid temperature, mixture enthalpy, mass flux, and bundle average pressure drop for the verification problems. All are less than 0.01% indicating that the integrity of the parallel solutions is barely harmed.

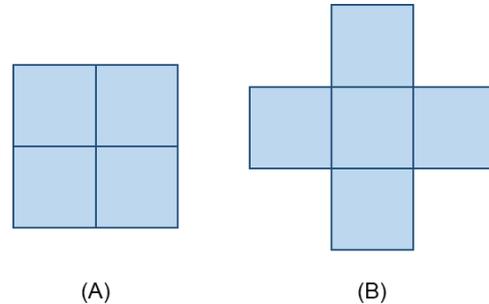


Fig. 4. Arrangement of assemblies for verification of ESCOT parallelization

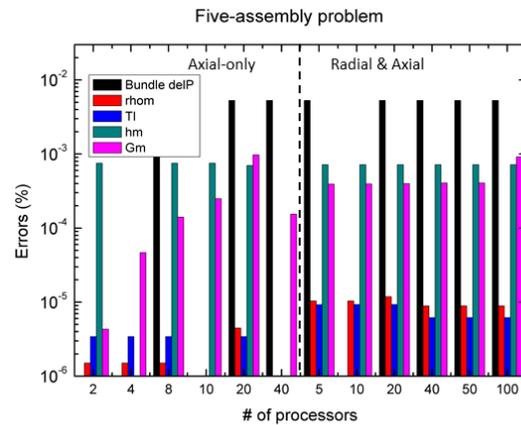
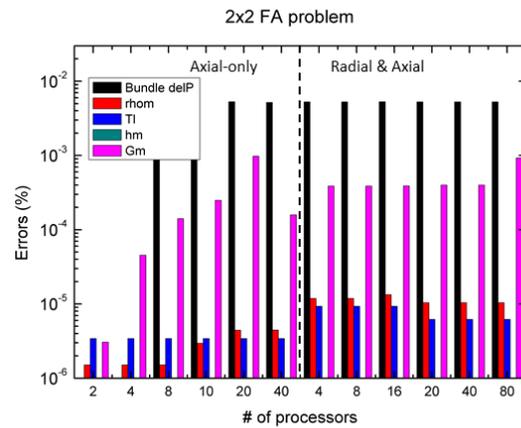


Fig. 5. Maximum errors of parallel solutions for verification problems

4. Parallel Performance Examination

In order to examine the parallel performance of ESCOT, conceptual problems with various sizes and a quarter core OPR1000 problem are solved.

4.1 N-by-N assembly problems

For the scalability analysis of the parallel execution of ESCOT, five conceptual problems were solved as increasing the size of problems – single assembly, 2x2, 3x3, 5x5, and 7x7 assembly. The same boundary conditions of the verification problem are applied. For the linear solver, the Block Jacobi preconditioned BiCGSTAB is used. The specification of the computing machine is Intel Xeon E5-2630 v4 2.20 GHz with InfiniBand, and the number of available processes on the test platform is 120 cores.

Fig. 6 presents the results of the scalability analysis. The upper figure is the scalability of the unidirectional domain decomposition. For the axial-only domain

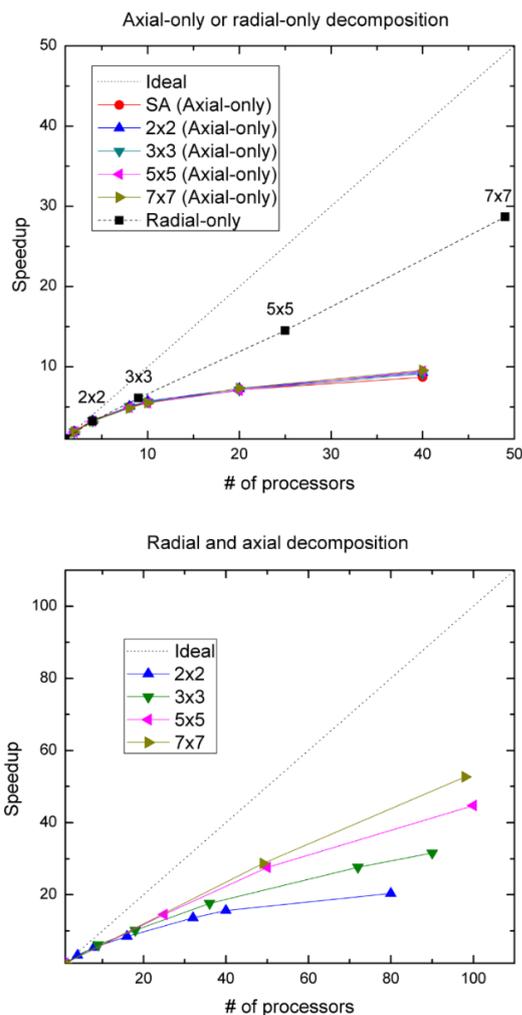


Fig. 6. Scalability of ESCOT parallel execution as increasing problem size

decomposition, the maximum number of processors is 40 which is same as the number of axial planes. The speedup is barely influenced by the problem size, and the curve is saturated early. In case of radial-only decomposition, the processors are assigned as one per single assembly. The speedup is linearly increased of about 60% efficiency, which is the characteristics of the weak scaling. The constant number of neighbors facing subdomains leads to a lower degradation of the parallel performance in the radial-only decomposition than in the axial-only decomposition.

Through the bidirectional decomposition, more processors are available as multiples of the number of assembly. The radial decomposition allows a better parallel performance as the problem size increases. It is expected that the fine speedup can be achieved with hundreds of processors for a full-core-size problem.

4.2 OPR1000 Quarter core

The parallel performance of ESCOT was examined to a real problem, a OPR1000 quarter core problem. The number of radial subdomains is 52 where 37 are full fuel assemblies, 14 are half-sized assemblies, and 1 is a quarter-sized. The number of subchannels is 11,569 and the active height is non-uniformly subdivided into 32 planes to yield 370,208 computational meshes. The pin power distribution shown in Fig. 7 was provided by the nTRACER [6] direct whole core calculation.

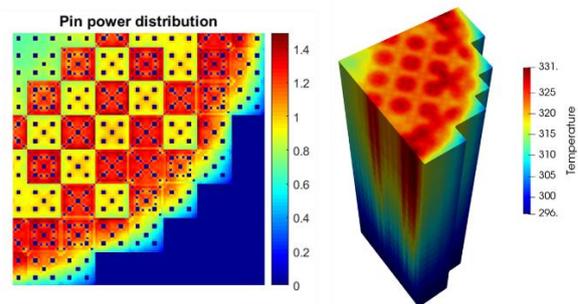


Fig. 7 nTRACER axially averaged radial pin power distribution (left) and ESCOT calculated coolant temperature (right) for OPR1000 quarter core problem

The comparison of the wall-clock time is given in Fig. 8. The computing time is reduced from 1,415 sec of the serial calculation to 30 sec with 104 processors. The bottom figure shows which computing section is the bottleneck as increasing the number of processors. The sections of solving scalar equation and momentum equation take few computing portion in the serial calculation, but they become considerable particularly in the axial-only parallel calculations due to the communication load. On the other hand, the sections of building linear systems and updating next time step variables are well-parallelized because they are naturally parallelizable or require a little communication.

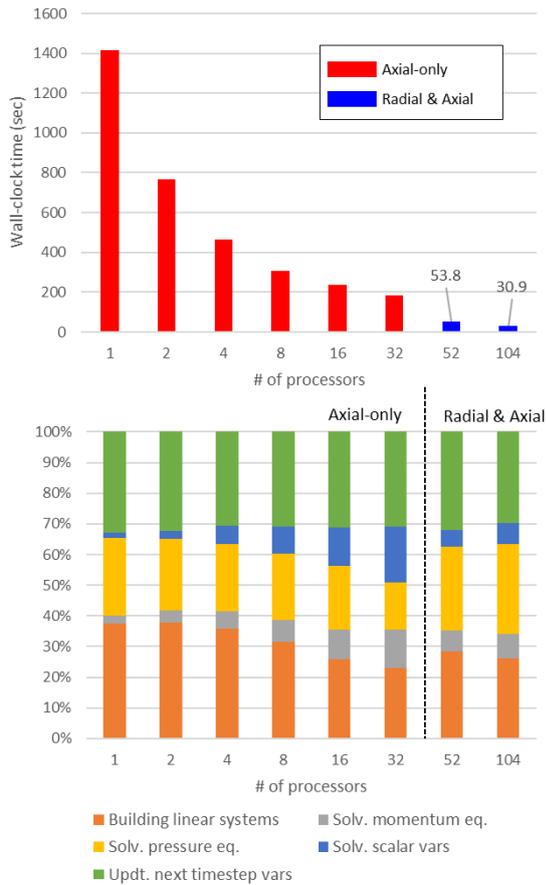


Fig. 8. Wall time (*top*) and portion of each computing section (*bottom*) for OPR1000 quarter core problem

5. Conclusions

A core T/H analysis code, ESCOT, is parallelized by applying the radial and axial domain decomposition with MPI and PETSc library for massively parallel executions. The available number of processors becomes larger and more flexible with the bidirectional domain decomposition. Moreover, through the scalability analysis, it turns out that the bidirectional domain decomposition can yield the improved parallel performance for large size problems. For a OPR1000 quarter core problem, the pin-wise T/H solutions in a core can be obtained in about 30 seconds with 104 processors. In the future, pin-wise multiphysics analyses will be performed with the efficient neutronics-T/H coupled platform using ESCOT.

ACKNOWLEDGEMENTS

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REFERENCES

- [1] J. Lee and H. G. Joo, "Preliminary Development of a Drift-Flux Model Based Pin-Resolved Core Thermal-Hydraulics Code for Dedicated Use in Efficient High-Fidelity Neutronics Coupled Calculations," *Trans. of the American Nuclear Society*, Las Vegas, NV, USA, Nov. 6-10, 2016.
- [2] R. Salko and M. Avramova, "COBRA-TF Subchannel Thermal-Hydraulics Code (CTF) Theory Manual-Revision 0," The Pennsylvania State University, 2015.
- [3] A. Facchini, J. Lee, and H. G. Joo, "Development and Validation of the Two-Phase Flow Analysis Capability of a Drift-flux Model Based Core Thermal-Hydraulics Code ESCOT," ICAPP 2019, Juan-les-pins, France, May 12-15, 2019.
- [4] R. K. Salko, R. C. Schmidt and M. N. Avramova, "Op Optimization and parallelization of the thermal-hydraulic subchannel code CTF for high-fidelity multi-physics applications," *Annals of Nuclear Energy*, vol. 84, pp. 122-130, 2015.
- [5] S. Balay, S. Abhyankar, M. F. Adams, J. Brown, P. Brune, K. Buschelman, L. Dalcin, A. Dener, V. Eijkhout, W. D. Gropp, D. Kauchik, M. G. Knepley, L. C. McInnes, K. Rupp, B. F. Smith, S. Zampini, H. Zhang, and H. Zhang, "PETSc Web page," <http://www.mcs.anl.gov/petsc> (2018).
- [6] Y. S. Jung et al., "Practical numerical reactor employing direct whole core neutron transport and subchannel thermal/hydraulic solvers," *Annals of Nuclear Energy*, vol. 62, pp. 357-374, 2013.