Parallelization of the SCALE Continuous-Energy Resonance Processing Module GEMINEWTRN

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INTRODUCTION

During a two-term internship at ORNL, funded in part by a U.S. Department of Energy Nuclear Energy Research Institute grant, a proof-of-principle code was developed to perform highly rigorous resonance self-shielding calculations for nontrivial geometries.

GEMINEWTRN¹ (Group and Energy Point-wise Methodology Implemented in NEWT for Resonance Neutronics) combines the pointwise (PW) solution of CENTRM² with the power and flexibility of NEWT's general-geometry two-dimensional (2-D) discrete-ordinates solver³ and can calculate the continuous-energy neutron spectra within large domains (e.g. an entire reactor fuel assembly).

Two-dimensional whole-assembly S_N calculations using continuous-energy data have been made feasible with the advent of large high-speed computer workstations, combined with the novel computational methods employed in both CENTRM and NEWT. However, even with these advantages, such calculations still require not only significant computational effort but also extensive amounts of computer memory. For a typical light-water-reactor assembly model, there are generally more than 30,000 energy points in the resonance-energy range. At each energy point, a transport sweep must be performed across the entire problem geometry domain, which typically contains on the order of 5000–10,000 spatial mesh cells.

In order to address this impediment to the practical application of GEMINEWTRN, parallel methods were applied to the code to provide a means for a more efficient solution mode by distributing both computational burden and memory requirements. It was recognized that GEMINEWTRN spends most of its computation time in transport sweeps at each energy point and that most of the memory is allocated to store the cumulative resonance integrals that are necessary for the PW scattering source calculation. Significant computational effort is also required for the calculation of the scattering source. Hence the first-generation parallelization of GEMINEWTRN sought to parallelize these facets of the iterative solution.

PARALLELIZATION

GEMINEWTRN is parallelized in the angular domain using the well-known MPI message-passing interface or OpenMP parallelization tool; for the scattering source calculation, GEMINEWTRN is parallelized in the spatial domain using MPI. The computational memory distribution is achieved by allocating the cumulative resonance integrals for the assigned spatial domain. Because the cumulative resonance integrals use the dominant amount of memory during the calculation, the memory burden on each processor can be reduced almost linearly to the number of processors.

To parallelize the transport sweeps within GEMINEWTRN, angular domain decomposition was introduced, in which the angular domain is divided into several angular subdomains, each of which is assigned to a different processor to perform transport sweeps. To balance the computational load, the same number of angles is assigned to each processor. Spatial domain decomposition was also implemented for the PW scattering source calculation. Because the size of the resonance integral evaluation is different for each isotope calculated, memory requirements are also different. Hence, the spatial distribution of resonance integral evaluations is based on mixtures, distributing the cells containing the same mixture onto individual processors as evenly as possible so that the resonance integrals associated with moment and submoment space will also be distributed evenly. All the variables related to the cumulative resonance integrals are defined only within each spatial subdomain. Thus, the required memory scales inversely with the number of processors used.

PARALLEL PERFORMANCE

To study the parallel performance of GEMINEWTRN, analysis was performed for a GE-12 full-assembly boiling-water-reactor (BWR) model, as illustrated in Fig. 1. In this model, there are more than 4000 computational cells, along with approximately 100 boundary surfaces and more than 32,000 energy points in the resonance-energy range. GEMINEWTRN spectra calculations were performed for this model to study the speedup performance, using S_4 angular quadrature (12 angles) and a P_1 scattering approximation in all mixtures. Calculations were performed on a parallel Linux cluster. Table I shows timing statistics for both the transport and scattering source calculations, along with the total speedup observed.

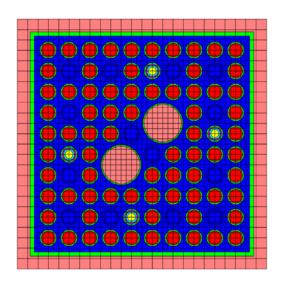


Fig. 1. GE-12 BWR assembly model.

TABLE I. Computation and Communication Times for GE-12 Analysis

Number of Processors	Transport Sweep			² Scattering Source			Total		
	¹ T _{Comm} (min)	³ T _{Comp} (min)	speedup/ (efficiency)	¹ T _{Comm} (min)	³ T _{Comp} (min)	speedup/ (efficiency)	¹ T _{Comm} (min)	³ T _{Comp} (min)	speedup/ (efficiency)
1		636.4			54.0			690.4	
2	6.5	314.1	2.03/(1.02)	2.8	29.7	1.82/(0.91)	9.3	343.8	2.01/(1.01)
4	11.0	163.1	3.90/(0.98)	3.1	16.5	3.28/(0.82)	14.1	179.6	3.84/(0.96)
6	12.2	113.4	5.61/(0.94)	3.8	13.8	3.91/(0.66)	16.0	127.2	5.43/(0.91)
12	13.8	65.2	9.86/(0.82)	4.7	9.9	5.04/(0.42)	18.5	75.1	9.19/(0.77)

¹Communication time.

CONCLUSION

Parallel methods have been implemented into GEMINEWTRN, with a considerable improvement in overall efficiency and problem tractability. The parallel approach scales well with the number of processors for the first few processors but drops off due to scattering source calculations with increasing numbers of processors. However, this reduction in efficiency is due in part to the simple nature of the fresh $\rm UO_2$ fuel used. When applied in burnup calculations with significant fractions of fission product nuclides, the scattering source efficiency will scale more linearly with the total number of processors.

Finally, because the 2-D transport solver in GEMINEWTRN is the same as that used in the lattice Physics code NEWT, a similar parallel method (for transport sweeps only) has been applied in NEWT, with highly efficient parallel gains observed.

REFERENCES

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²Scattering source calculation.

³Computation time.

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