Scientific Application Project – *"Tera-scale computation of wave-plasma interactions in multidimensional fusion plasmas"*

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Summary

This Scientific Application Project (SAP) assists the fusion scientists in exploring and implementing efficient algorithms for modeling the response of fusion plasma to radio frequency (RF) waves in two-dimensional tokamak and fully three-dimensional stellarator geometries on high performance computers. The project has optimized advanced algorithms to speedup full-wave spectral codes, in some cases by several orders of magnitude. This enabled the study of new regimes of wave physics that previously could only be treated in one dimension or with approximate techniques, and to carry out multiple code runs at high resolution for scientific case studies where it was previously not feasible.

There is great potential for electromagnetic wave techniques to exert control of fusion plasma by means of localized heating, current drive, flow drive and energetic particle production. Fundamental understanding of these interactions of radio frequency (RF) waves on high temperature fusion plasma is of major importance. This Scientific Application Project (SAP) collaborates with fusion scientists on the project "Tera-scale computationa of wave-plasma interactions in multidimensional fusion plasmas" as part of the Scientific Discovery Through Advanced Computing (SciDAC) program. The goal of the effort is to ensure that the best available mathematical algorithms and computer science techniques are employed. Successful development and optimization of these full-wave simulation codes would enable more accurate treatment of plasma with large (non-Maxwellian) energetic particle populations.

A suite of all-orders spectral algorithm (AORSA) full-wave codes has been developed to model the wave-plasma interactions. Full-wave models are needed because traditional ray tracing model cannot fully capture certain characteristics in the plasma such treatment of realistic antenna spectra, plasma cutoffs, or mode conversion layers, nor does ray tracing include large scale coherent effects such as diffraction, interference, and wave focusing. Recent full-wave codes use a superposition of Fourier modes for representing the electric fields and currents. This formulation requires the solution very large dense complex linear systems. The project has

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implemented a new formulation that transforms the linear system from Fourier space back to configuration space. This allows the solution matrix to be condensed by eliminating all boundary points outside the plasma. The savings lead to an over 100 fold speed up in the ScaLAPACK parallel linear solver and a overall 27 fold speedup in a three-dimensional calculation.

The improved performance allows consideration of better physics such as a general non-Maxwellian distribution for particles. Conductivity tensor for a Maxwellian distribution can be evaluated using modified Bessel functions and special Z functions, whereas more costly evaluations of Cauchy principal value integrals,

$$PV\int_a^b \frac{f(x)}{(x-c)}dx = \lim_{\varepsilon\to 0}\int_a^{c-\varepsilon}\frac{f(x)}{(x-c)}dx + \int_{c+\varepsilon}^{b}\frac{f(x)}{(x-c)}dx$$

are needed for the general non-Maxwellian case.

The AORSA codes have been ported to the CRAY X1 vector supercomputer to take advantage of the faster processing capabilities. Performance optimization to take full advantage of the CRAY vector architecture required new algorithms in the fast evaluation of Cauchy principal value (PV) integrals, and modified Bessel functions. Instead of using a general quadrature package that cannot be easily vectorized, the new algorithm represents a function $f(x)$ using a spline approximation. Over each sub-interval, the piecewise polynomial is re-expressed as $f(x) = d_0 + d_1(x-c) + d_2(x-c)^2$ and the PV is evaluated using

$$\int_a^b \frac{f(x)}{(x-c)}dx = \int_a^b \{d_0(x-c)^{-1} + d_1 + d_2(x-c)\}dx$$

and $\int_a^b (x-c)^{-1}dx = \ln(b-c) - \ln(a-c)$.

The new vectorized version is over 10 times faster as compared to using the quadrature package. The evaluation of modified Bessel function was originally based on a series expansion with truncation based on an error tolerance. This formulation was efficient on a scalar processor such as the IBM Power3 but inappropriate for vector machines since it introduced unavoidable data dependencies. The new formulation batches multiple evaluations of modified Bessel function and uses an approximation by min-max Chebyshev polynomials. These Chebyshev polynomials can be evaluated using very efficient level 3 BLAS matrix multiply routines. Table 1 shows the run time (in minutes) of several modules in AORSA based on the non-Maxwellian integral formulation. This vectorized version of AORSA on the CRAY X1 is about 7 times faster than the version on the NERSC IBM Power3 machine.

128 processor	*NERSC (power3)*	*Cheetah (power4)*	*Phoenix (CrayX1)*
Matrix load	207.7min	37.3min	13.7min
ScaLAPACK	8.5min	3.9min	2.0min
Plasma current	151.9min	45.7min	16.4min
absorption	86.3min	39.7min	31.4min
Total cpu	456min	127min	64min

Table 1: Performance of AORSA on supercomputers

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