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Numerical Tokamak Turbulence Project (OFES Grand Challenge)

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Research Objectives:

The primary research objective of the Numerical Tokamak Turbulence Project (NTTP) is to develop a predictive ability in modeling turbulent transport due to drift-type instabilities in the core of tokamak fusion experiments, through the use of three-dimensional kinetic and fluid simulations and the derivation of reduced models.

Significance of Research:

The NTTP simulations are being used to produce linear and nonlinear calculations of drift-type instabilities in realistic tokamak equlibria, which are leading to a deeper understanding of anomalous transport in current experiments and to improving their performance. This simulation work is providing a basis for reduced transport models that fit current experimental databases and from which it is hoped that performance in future experiments can be reliably predicted and optimized. As controlling the energy transport has significant leverage on the performance, size, and cost of fusion experiments, reliable NTTP simulations can lead to significant cost savings and improved performance in future experiments.

Computational Approach:

Two main classes of three-dimensional initial-value simulation algorithms, gyrokinetic (GK) and gyro-Landau-fluid (GLF), are being applied to the simulation of tokamak turbulent core transport. Most of the GK simulations are based on particle-in-cell (PIC) methods for the self-consistent solution of Poisson's (or Maxwell+Poisson in electromagnetic extensions) equation(s) (reduced to a quasi-neutrality relation for the Poisson equation) and plasma equations of motion, and domain decomposition methods to run efficiently in parallel on the T3E and other parallel computers. In addition to these PIC codes, a widely-used, linear electromagnetic Eulerian (5-D) GK code has been extended to describe nonlinear systems. The GLF algorithm is based on an alternative solution of the fundamental GK and quasi-neutrality equations, in which fluid moment equations are solved instead of particle equations. The GLF simulations have been performed on massively parallel computers, particularly the T3E at NERSC. Both flux-tube, i.e., toroidal annulus, and global toroidal GK and GLF simulations are being performed to study tokamak turbulence.

The NTTP Grand Challenge is comprised of a suite of gyrokinetic and gyrofluid codes (flux-tube and global) which are summarized in the following. The code developers are predominantly Ph.D.'s in computational plasma physics and a few graduate Ph.D students. For more information on the NTTP please see:

http://www.acl.lanl.gov/GrandChal/Tok/tokamak.html
http://www.er.doe.gov/production/cyclone/

I. Gyrokinetic Turbulence Simulation Codes

Global Gyrokinetic

**UCAN (UCLA-U. Alberta, Canada) Global Toroidal Low-Noise Gyrokinetic Particle Code

Rick Sydora Viktor Decyk Jean-Noel Leboeuf

This is a global, three dimensional, toroidal, low noise, gyrokinetic particle code which calculates plasma turbulence at the core of magnetic confinement fusion devices such as tokamaks. It uses the delta-f method to integrate the characteristics of the gyrokinetic Vlasov equations over the entire plasma cross section. It moves either ions or ions and bounce-averaged trapped electrons. It employs cartesian geometry and the gyrokinetic Poisson's equation, needed to calculate the electrosttaic forces to which the particles respond, is solved using Fast Fourier Transforms. It uses domain decomposition in the toroidal direction and parallelization is accomplished through UCLA's own MPI-based PLIB library which contains a whole array of particle management routines. The gyrokinetic code is written in Fortran 77 and amounts to close to 5000 lines distributed over about 20 subroutines. The gyrokinetic code can run serially or on any parallel computer supporting MPI.

major code characteristics:
number of lines of code: 5000
number of subroutines: 20 languages: F77
standard mathematical algorithms used: parallel FFT's
standard communications packages used: MPI

general frameworks used: PLIB library; a set of particle management routines in which is embedded 1D domain decomposition in the toroidal direction with MPI for message passing

computers on which the code runs: T3E, Cray PVP, IBM SP2, any parallel computer supporting MPI

Documentation:

R. D. Sydora, "Toroidal gyrokinetic particle simulations of core fluctuations and transport", Physica Scripta, 52, 474 -480 (1995).

R. D. Sydora, V. K. Decyk, and J. M. Dawson, "Fluctuation-induced heat transport results from a large global 3D particle simulation model", Plasma Physics and Controlled Fusion, 38 (1996) A281-A294.

****Orb**

S.E. Parker, C. Kim, Y. Chen , University of Colorado, Boulder
W.W. Lee,Princeton Plasma Physics Laboratory
J.C. Cummings, LANL
R.A. Santoro, NRL M. Tran, CRPP-EPFL
V. Decyk, UCLA

Physics capabilities: 3D Toroidal, global, nonlinear, electrostatic with adiabatic electrons, numerical MHD equilibrium, gyrokinetic ions, multiple ion species.

major code characteristics:
number of lines of code: 8000 number of subroutines: 50 languages: F90
standard mathematical algorithms used: parallel FFT's
tandard communications packages used: MPI (1D Domain decomposition).

general frameworks used: PLIB library (UCLA)

computers on which the code runs: T3E, Cray PVP, SGI Origin

documentation:

****GTC**

Z. Lin, W.W. Lee, W.M. Tang, Princeton Plasma Physics Laboratory

Physics capabilities: 3D Toroidal, global, nonlinear, electrostatic, gyrokinetic-delta-f particle ions; adiabatic electrons; Can use idealized equilibria or interface to and general tokamak and 3D (e.g., stellarator) equilibria. Momentum-, energy- and Maxwellian-preserving ion-ion collision operator (important to dynamics of zonal flows). Field-line following coordinates to obtain high resolution for a given number of grid cells and low noise for given number of particles.

major code characteristics:

number of lines of code: 4000 lines of F90 code (GTC), 2000 lines of IDL procedures (visualization),
number of subroutines: 30 languages: F90
numerical methods: non-spectral Poisson solver
standard mathematical algorithms used: ??
standard communications packages used: MPI [1-D domain-decomposition]

general frameworks used: ??

computers on which the code runs: T3E, Cray PVP, Oriing2000

****GTC++**

Z. Lin, W.W. Lee, Princeton Plasma Physics Laboratory T.J. Williams, J.A. Crotinger, LANL

Physics capabilities: 3D Toroidal, global, nonlinear, electrostatic, gyrokinetic-delta-f particle ions; adiabatic electrons; Can use idealized equilibria or interface to and general tokamak and 3D (e.g., stellarator) equilibria. Momentum-, energy- and Maxwellian-preserving ion-ion collision operator (important to dynamics of zonal flows). Field-line following coordinates to obtain high resolution and low noise for given number of particles. We wrote the code using (and extending) the POOMA C++ class library. Currently, it supports analytical equilibria, but is ready for extension to more complex geometries such as experimental or computed equilibria---the computational framework and many required mechanisms are already in place.

major code characteristics:

number of lines of code: 7200 number of classes (excluding POOMA library classes): 15
number of subroutines (excluding class member functions): 10 languages: C++
standard mathematical algorithms used: vendor and public-domain 1D FFT's
standard communications packages used: MPI (encapsulated by POOMA) [1-D, 2-D, or 3-D domain-decomposition]
general frameworks used: POOMA

computers on which the code runs: T3D/E, SGI Origin 2000, most serial UNIX workstations, Mac and Windows PC's

Code documentation: Online presentation from APS DPP 1998 meeting, at POOMA website.

Gyrokinetic (GK) flux-tube

****PG3EQ**

A.M. Dimits, B.I. Cohen, W.M. Nevins, D.E. Shumaker, Lawrence Livermore National Laboratory T. Williams, Los Alamos National Laboratory

Physics capabilities: 3D Toroidal, flux-tube and flux-ribbon (or "wedge" - with global profile variation effects) geometry, nonlinear, electrostatic, gyrokinetic ions; adiabatic electrons; Idealized and general tokamak equilibria; can include any equilibrium velocity shear components; multiple-ion-species dilution model for beams and impurities.

Numerical aspects: Quasiballooning representation (~O(10) more efficient than "field-line-following coordinates" at given resolution and noise level); delta-f-particle ions

Computational aspects: 2D Domain decomposition for optimal parallelism.

Major code characteristics:
number of lines of code: 18,300 lines F90 source, 2,300 lines C, 10,000 lines IDL procedures (+ a small amount of PV-Wave procedures being ported to IDL).
number of subroutines: 64 F90; 20 C; 40 IDL and PV-Wave; 4 AVS.

languages: F90 for code source, C for MP wrappers; F90, PV-Wave, IDL, and AVS for postprocessing and graphics (IDL is the most important of these).
standard mathematical algorithms used: parallel FFT's, parallel complex tridiagonal matrix solves.
standard communications packages used: PVM and MPI (2D Domain decomposition), NetCDF for I/O.
general frameworks used: MPFUNCS - message passing wrapper library which circumvents the need to explicitly change message-passing calls when porting between machines or between message-passing/communication libraries.

computers on which the code runs: T3E, Cray PVP, DEC-alpha SMP.

documentation: HTML documents on the use of the gyrokinetic code; Some of the IDL procedures operate through an intuitive GUI. Also, the following publications and references therein.

A. M. Dimits, T. J. Williams, J. A. Byers, and B. I. Cohen, Phys. Rev. Lett. 77, 71 (1996).

A. M. Dimits, B. I. Cohen, N. Mattor, W. M. Nevins, and D. E. Shumaker, S. E Parker and C. Kim, Proceedings of the 17th. IAEA Fusion Energy Conference (paper IAEA-F1-CN-69/TH1/1, accepted for publicaton in Nuclear Fusion).

****CU Flux-Tube Gyrokinetic Code**

S.E. Parker, C. Kim, Y. Chen , University of Colorado, Boulder

Physics capabilities: 3D Toroidal, flux-tube and flux-ribbon (or "wedge" - with global profile variation effects) geometry, nonlinear, electromagnetic, gyrokinetic ions, drift-fluid electrons.

Numerical aspects: field-line-following coordinates.

major code characteristics:
number of lines of code: 7000
number of subroutines: 35 languages: F90
standard mathematical algorithms used: parallel FFT's standard communications packages used: MPI (1D Domain decomposition).

computers on which the code runs: T3E, Cray PVP, SGI Origin Brief summary of documentation:

****GS2**

W. Dorland, University of Maryland
M. Kotschenreuther, U. Texas
Q.P. Liu, Motorola

Physics capabilities: 5D, electromagnetic (delta A_parallel and delta B_parallel), toroidal, flux-tube, nonlinear, gyrokinetic description of both Maxwellian (ions and/or electrons) and slowing-down species (such as helium ash); momentum-conserving Lorentz collision operator; uses general axisymmetric equilibria (specified analytically or numerically). Non-axisymmetric calculations require interface to numerically specified equilibria.

Numerical aspects: 5-D Eulerian phase-space scheme; object-oriented design; 4-D domain decomposition; implicit linear dynamics, including implicit treatment of electromagnetic waves; explicit pseudo-spectral predictor-corrector integration of the nonlinear terms; parallelism implemented mainly with MPI; SHMEM optimizations available.

number of lines of code: 50,000
number of subroutines: ~50 languages: Fortran 90
standard communications packages used: MPI, SHMEM (both optional) [4-D domain-decomposition on parallel computers/networks]
general frameworks used: object-oriented design; significant fraction of code shared with Gryffin and other non-NTTP codes.

computers on which the code runs: any serial computer with Fortran-90 compiler; any parallel computer with Fortran-90 compiler and MPI library.

Support and documentation: Original documentation is in

Kotschenreuther, Rewoldt and Tang, CPC, Vol. 88, (1995) 128.

Linear component of code is one of two standard codes in the world for GK stability analysis of experimental data [the other is Rewoldt's FULL code (PPPL)] and has been used for dozens of publications.

Current source code (for linear component) is available on-line at http://kendall.umd.edu/~bdorland/GS2

Free on-line support provided for all users. User group presently includes 17 scientists from the US, Japan, and Europe.

Documentation of more recent nonlinear routines is under development.

**Skeleton PIC Code

Viktor K. Decyk, UCLA

This is a simple 3d skeleton particle-in-cell code designed for exploring and evaluating new computer architectures and algorithms. It contains the critical pieces needed for depositing charge, advancing particles, and solving the field. The code moves only electrons, with periodic electrostatic forces obtained by solving Poisson's equation with Fast Fourier Transforms. Since the code is primarily a research tool, it is constantly evolving and there are many versions. Successful algorithms are incorporated into other production codes.The current version is based on MPI, the next version will probably be based on OpenMP. The base code contains about 4,000 lines of Fortran77, and about 20 subroutines. The current code can run either serially or on any parallel computer which supports MPI.

major code characteristics:
number of lines of code: 4000
number of subroutines: 20 languages: F77
standard communications packages used: MPI

computers on which the code will run: The serial code will run on almost anything, and the parallel code will run on anything having MPI.

Documentation:

The code and algorithms used are described in following publications:

P. C. Liewer and V. K. Decyk, "A General Concurrent Algorithm for Plasma Particle-in-Cell Simulation Codes," Journal of Computational Physics 85, 302 (1989). V. K. Decyk, "Skeleton PIC codes for parallel computers," Computer Physics Communications 87, 87 (1995).

V. K. Decyk, S. R. Karmesin, A. de Boer, and P. C. Liewer, "Optimization of particle-in-cell codes on RISC processors," Computers in Physics 10, 290 (1996).

V. K. Decyk, H. Naitou, and S. Tokuda, "Particle-in-cell simulation on the Fujitsu VPP500 parallel computer", Supercomputer 66, vol. XII-4, 28 (1996).

II. Gyro-Landau-fluid Turbulence Simulation Codes

The GLF algorithm is based on an alternative solution of the fundamental GK and quasi-neutrality equations, in which fluid moment equations are solved instead of particle equations. The GLF simulations have been performed on massively parallel computers, particularly the T3E, Cray PVP at NERSC.

Global Gyro-Landau-Fluid (GLF) code.

**ITDGT, Global toroidal nonlinear Landau fluid code for ion temperature gradient driven turbulence(ITGDT) in tokamaks

J.N. Leboeuf, UCLA;
V. Lynch, Oak Ridge National Laboratory

Physics capabilities: 3D Toroidal, global, nonlinear, electrostatic, gyro-Landau-fluid ions; adiabatic electrons, real geometry.

Numerical aspects: Finite differences in the radial direction, Fourier expansion in poloidal and toroidal directions, time implicit treatment of the linear terms (matrix operations), time explicit treatment of the nonlinear terms (mode convolutions)

Computational aspects: parallelization effected over the number of toroidal modes for the matrix solves and over the number of radial grid points for the convolutions (which are performed analytically)

major code characteristics:
number of lines of code: 20000
number of subroutines: 200 languages: F90,
standard mathematical algorithms used: block tri-diagonal matrix solves standard communications packages used: PVM, MPI (1D Domain decomposition).

general frameworks used: BTMS Block Tri-diagonal Matrix Solver from Hindmarsh (LLNL)

computers on which the code runs: T3E, Cray PVP, SGI Origen

Brief summary of documentation:

L. Garcia , J. D. Alvarez, J. N. Leboeuf, V. E. Lynch, and B. A. Carreras, "Nonlinear full torus calculations of resistive-pressure-gradient-driven turbulence and ion-temperature-gradient-driven turbulence in toroidal geometry," Plasma Physics and Controlled Nuclear Fusion Research 1998, to be published, IAEA, Vienna (1999)

J. N. Leboeuf, V. E. Lynch, B. A. Carreras, J. D. Alvarez, and L. Garcia, "Full-Plasma Cross Section Landau Fluid Calculations of Ion Temperature Gradient-Driven Turbulence in Tokamaks," Paper 1B5, p. 47-50, Proceedings of the 16th International Conference on Numerical Simulation of Plasmas, 10th - 12th February, 1998, Goleta, California.

V. E. Lynch, J. N. Leboeuf, B. A. Carreras, J. D. Alvarez, and L. Garcia,"Plasma turbulence calculations on the CRAY T3E", Supercomputing '97, San Jose, California, November 15-21, 1997, IEEE Computer Society Press, Los Alamitos, CA, 1997. Published electronically
as: http://www.supercomp.org/sc97/proceedings/TECH/LYNCH/INDEX.HTM

Gyro-Landau-Fluid (GLF) Flux-Tube

****Gryffin**

M. Beer, G.W. Hammett, P. Snyder, Princeton Plasma Physics Laboratory
W.D. Dorland, University of Maryland
S. Smith, Los Alamos National Laboratory

Physics capabilities: 3D Toroidal, flux-tube, nonlinear, electrostatic or electromagnetic, gyro-Landau-fluid ions; adiabatic or bounce-aveaged drift-kinetic electrons; Idealized and general tokamak equilibria

Numerical aspects: field-line-following coordinates

major code characteristics:
number of lines of code: 20000 (including source and diagnostics and many comments, excluding another 4000 lines of a public-domain spline package and 7700 lines of source and comments for a Fortran90 package for parallel communications layered over MPI/SHMEM, which is shared among multiple codes)
number of subroutines: 150 (plus Fortran90 parallel communications package, etc.)
languages: F90 (and IDL for some postprocessing)
standard mathematical algorithms used: parallel FFT's
standard communications packages used: MPI, SHMEM (3D Domain decomposition).

computers on which the code runs: T3E, Cray PVP, LINUX boxes, SGI Origin 2000

Brief summary of documentation: Gryffin has a user's documentation directory of files including a history of code changes, test suite (sample inputs and outputs) and a help file.