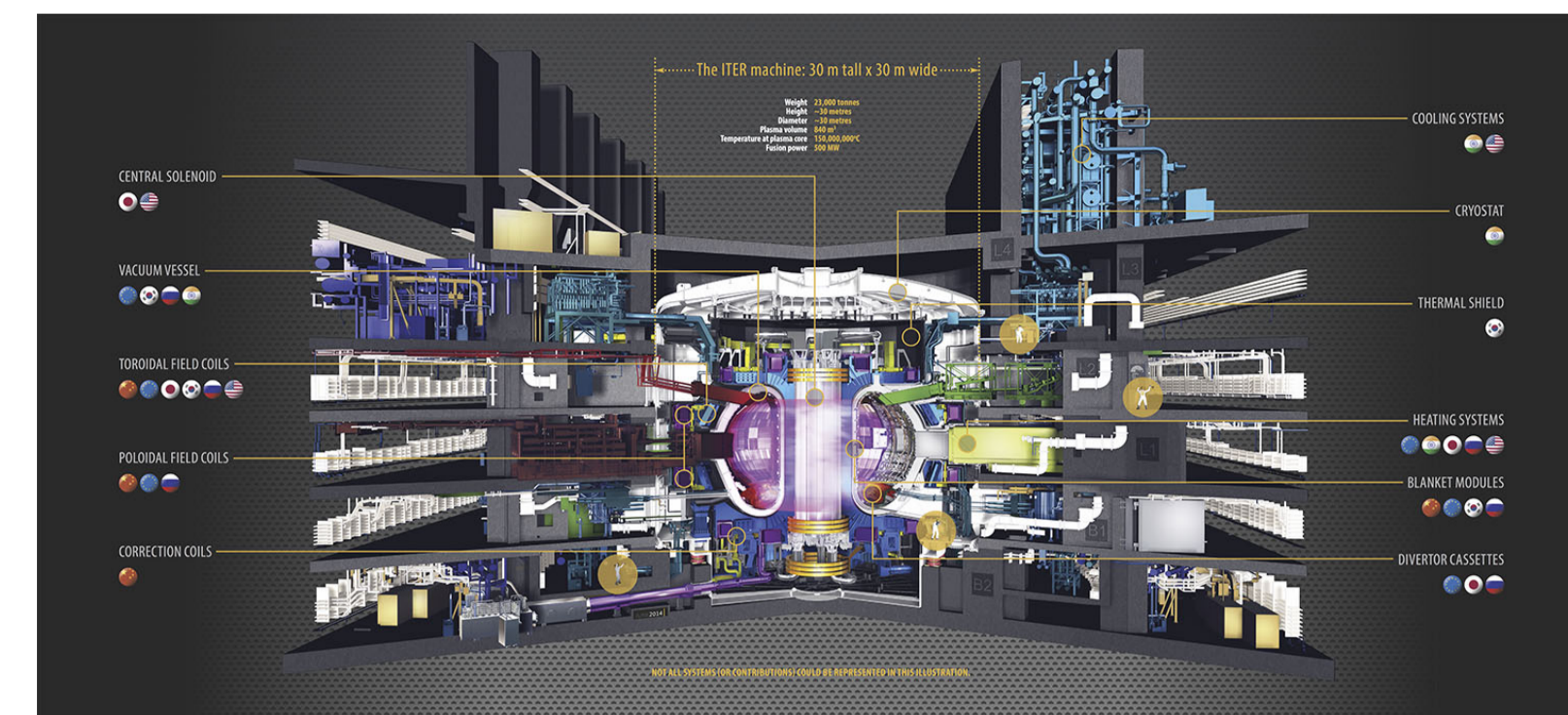
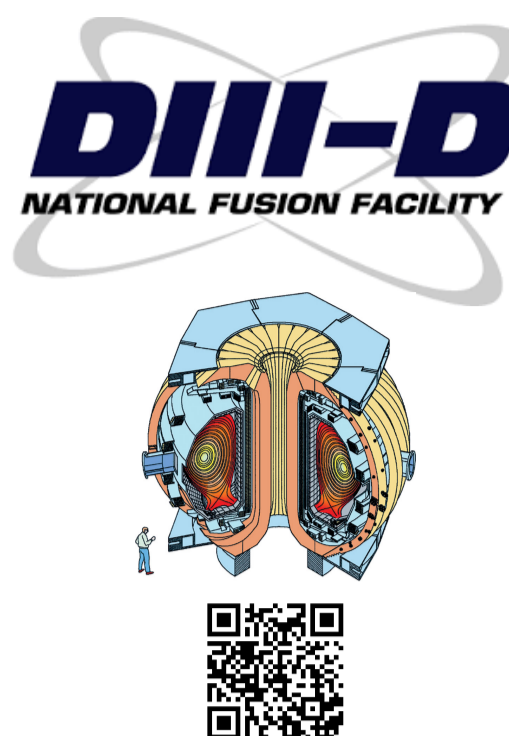
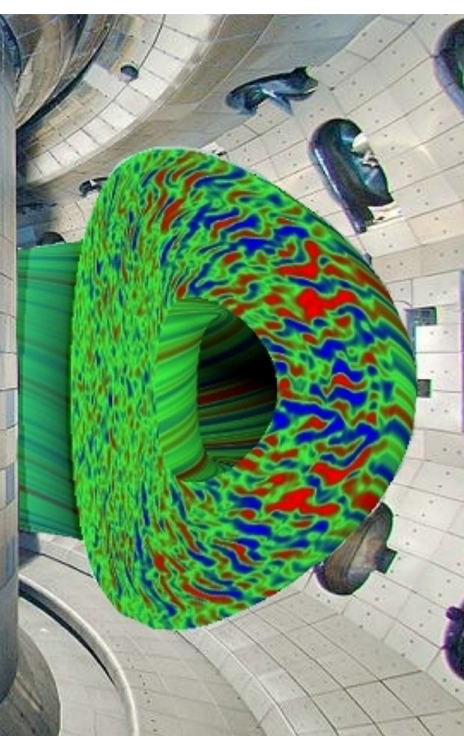


# Kernel-Based and Total Performance Analysis of CGYRO on 4 Leadership Systems

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## Fusion plasma as a low-carbon energy source

The US and global economies increasingly depend on reliable sources of energy. In coming decades, these sources must become increasingly low-carbon to mitigate the risks of climate change. Thus, the challenge to harness the virtually inexhaustible potential of fusion energy is being pursued in a coordinated worldwide effort. In parallel with a vibrant global research program (based primarily on the toroidal magnetic confinement, or tokamak, concept), numerical simulation serves as a powerful tool for accelerating progress. Simulations are used to validate basic theory, plan experiments, interpret results on present devices, and ultimately to design future devices. While the *long-term* goal of fusion simulation is to provide the scientific basis for a demonstration reactor, a *near-term* goal is to refine our understanding of physics issues associated with burning plasmas. This simulation capability relies on high-performance computing, enabling researchers to obtain key insights from fundamental physical models.



## CGYRO, a novel fusion plasma solver

CGYRO is an Eulerian gyrokinetic solver designed and optimized for collisional, electromagnetic, multiscale fusion plasma simulation. It is written in Fortran 2008 and was designed to be suitable for next-generation computational systems that require high levels of parallel concurrency. The implementation combines 15 years of algorithmic lessons learned from GYRO, together with an array distribution scheme and loop structure that targets modern multicore and accelerated (GPU) architectures. CGYRO was designed for operation on Petascale systems, and employs MPI to split the problem over a potentially very large number of compute processes. Moreover, the in-process parallelization scheme for most kernels employs cache-aligned data arrays, OpenMP and OpenACC parallelized loops and vectorization-friendly operations.

### The gyrokinetic model

The nonlinear, electromagnetic GK equations specify 5D particle distributions for electron and multiple ion species:

$$\frac{\partial \tilde{h}_a}{\partial t} + A(\tilde{h}_a, \tilde{\Psi}_a) + B(\tilde{h}_a, \tilde{\Psi}_a) = 0, \quad (8)$$

where the subscript  $a$  is the species index, and the tilde indicates a Fourier space quantity. The spatial coordinates are

$$\begin{aligned} k_x &\rightarrow \text{radial wavenumbers} \\ k_y &\rightarrow \text{binormal wavenumbers} \\ \theta &\rightarrow \text{field-line coordinate} \end{aligned} \quad (2)$$

where  $k_x^2 = k_x^2 + k_y^2$ , and the velocity-space coordinates are

$$\xi = v_{\parallel}/v \rightarrow \text{cosine of the pitch angle } \in [-1, 1] \\ v \rightarrow \text{speed } \in [0, \infty] \quad (5)$$

Because of the use of twisted fieldline coordinates, the radial wavenumbers  $k_x$  are dependent on  $\theta$  and  $k_y$ . For this reason, it is convenient to define a primitive radial wavenumber  $k_x^0$  (the value of  $k_x$  at  $\theta = 0$ ) that can be directly quantized (in CGYRO, we write  $k_x^0 = 2\pi p/L$  where  $p$  is an integer, and  $L$  is the radial domain size). The spectral representation in terms of  $(k_x, k_y)$  is key to the arbitrary wavelength formulation and diagonalizes the gyroviscosity dynamics.

The GK equations are written in terms of an electromagnetic field potential  $\tilde{\Psi}_a$ , defined as

$$\tilde{\Psi}_a = J_{\parallel a}(k_x, k_y, \theta, \xi, v), \quad (7)$$

where  $m_a$ ,  $z_a$  and  $\rho_a$  are the species mass, charge and gyroradius. Above,  $(\delta \tilde{h}_a, \delta \tilde{A}_a, \delta \tilde{B}_a)$  are the electrostatic, transverse electromagnetic, and compressional electromagnetic potentials respectively, computed via coupling with the Maxwell equations. The Bessel functions  $J_0$  and  $J_1$  in Eq. (7) arise from gyroaveraging. This simply, compact representation of the field potential  $\tilde{\Psi}_a$  (and the Maxwell equations that we will write shortly) is only possible using a spectral wavenumber expansion. In terms of  $\tilde{\Psi}_a$ , the GK equation for species  $a$  is written symbolically as

$$\frac{\partial \tilde{h}_a}{\partial t} + A(\tilde{h}_a, \tilde{\Psi}_a) + B(\tilde{h}_a, \tilde{\Psi}_a) = 0, \quad (8)$$

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## CGYRO kernels

CGYRO can be split in four logical kernels: **str**, **n1**, **field** and **coll1**. Each simulation performs many iterations of the above, with MPI communication required to maintain a global view. The problem has been formulated to intentionally push most of the computation to the FFT-based n1 kernel.

Kernel type	Compute operation	Comm. operation	MPI comm.
<b>str</b>	loop	MPI_ALLREDUCE	1
<b>n1</b>	FFT	MPI_ALLTOALL	2
<b>field</b>	loop	MPI_ALLREDUCE	1
<b>coll1</b>	matrix-vector multiply	MPI_ALLTOALL	1

## MPI problem splitting

CGYRO operates on a 6 dimensional grid (3D space + 2D velocity + 1D species), which it splits using two orthogonal MPI communicators. MPI communicator 2 size is fixed by the problem size; it is always the value of N\_TOROIDAL (i.e.  $k_y/2$ ). All the other dimensions are then lumped together, and can be distributed along the MPI communicator 1.

## Benchmarked configurations

CGYRO can be used for both small-scale simulations of the plasma core and large-scale, multiscale simulations required for accurately describing the pedestal region. And anything in between. We present the benchmark results of two test cases that are broadly representative of small multiscale simulations.

Parameter	N_RADIAL	2 x N_TOROIDAL	N_THETA	N_XI	N_ENERGY	N_SPECIES
<b>Mesh var.</b>	$k_x$	$k_y$	$\theta$	$\xi$	$v$	$a$
<b>n103</b>	512	2 x 64 = 128	32	24	8	3
<b>n104</b>	512	2 x 128 = 256	48	24	8	4

## Tested Leadership Systems



	Stampede 2 Skylake	Stampede 2 KNL	Cori	Piz Daint	Titan
<b>CPU model</b>	2 x Xeon Platinum 8160	Xeon Phi 7250	Xeon Phi 7250	Xeon E5-2690 v3	Opteron 6274
<b>GPU model</b>	-	-	-	Tesla P100	Tesla K20x
<b>Threads/node</b>	96	272 (128 used)	272 (128 used)	24 (12 used) + 3584	16 + 2688
<b>TFLOPS/node</b>	3.5	3.0	3.0	4.5 (0.5+4.0)	1.5 (0.2+1.3)
<b>Max. Nodes</b>	1736	4200	9668	5320	18688
<b>Interconnect</b>	Intel Omni-Path	Intel Omni-Path	Cray Aries	Cray Aries	Cray Gemini
<b>Net. Topology</b>	Fat Tree	Fat Tree	Dragonfly	Dragonfly	3D Torus
<b>Compiler</b>	Intel Fortran 17	Intel Fortran 17	Intel Fortran 17	PGI Fortran 17	PGI Fortran 17
<b>FFT library</b>	Intel MKL	Intel MKL	FFTW v3.3.6	cuFFT	cuFFT
<b>MPI library</b>	MPICH v7.6	MPICH v7.6	Cray MPICH v7.6	Cray MPICH v7.6	Cray MPICH v7.6



## Collisionless step – Kernels str, n1 and field

The collisionless step operates primarily on the spatial dimensions and is distributed in the velocity dimensions. The collisionless step requires solution of the equation:

$$\frac{\partial \tilde{h}_a}{\partial t} + A(\tilde{h}_a, \tilde{\Psi}_a) = 0, \quad (1)$$

and uses an explicit time advance (RK4). We write the collisionless term symbolically as:

$$A(\tilde{h}_a, \tilde{\Psi}_a) = -i(\Omega_{\text{parallel}} + \Omega_{\text{binormal}}) \tilde{h}_a - i\Omega_{\text{drift}} \tilde{\Psi}_a \\ - \frac{c}{B} \sum_{k_x, k_y} (\mathbf{b} \cdot \mathbf{k}'_x \times \mathbf{k}'_y) \tilde{\Psi}_a(\mathbf{k}'_x, \mathbf{k}'_y, \xi, v), \quad (2)$$

The linear terms in  $A(\tilde{h}_a, \tilde{\Psi}_a)$  include the parallel streaming along the field line,

$$-i\Omega_{\text{parallel}} = \frac{v_{\parallel}}{w} \frac{\partial}{\partial \xi}, \quad (3)$$

the drift motion perpendicular to the field line,

$$-i\Omega_{\text{drift}} = i k_x \rho_a \frac{v^2}{2v_{\text{th}a}} \left( \mathbf{b} \times \frac{\nabla B}{B} + \xi \frac{\partial \mathbf{b}}{\partial \xi} \right) \cdot \nabla_{\mathbf{v}}, \quad (4)$$

and instability drive from equilibrium density and temperature gradients

$$-i\Omega_{\text{binormal}} = -i k_y \rho_a \frac{v^2}{2v_{\text{th}a}} \left( \frac{d \ln n_a}{dr} + \frac{d \ln T_a}{dr} \left( \frac{v^2}{2v_{\text{th}a}^2} - \frac{3}{2} \right) \right), \quad (5)$$

Here  $w = c/(c_s B/a)$  is an effective velocity (where  $c_s$  is the Jacobian determinant),  $\mathbf{b} = \mathbf{B}/B$ ,  $\rho$  is the total pressure,  $v_{\text{th}a} = \sqrt{T_a/m_a}$  is the thermal speed,  $\rho_a = v_{\text{th}a}/\Omega_a$  is the gyroradius,  $\rho_a = c/\Omega_a B_{\text{min}}$  is the effective ion-sound gyroradius, and  $k_{\parallel}$  is related to  $k_x$ . The linear terms in  $A(\tilde{h}_a, \tilde{\Psi}_a)$ , namely  $\Omega_{\text{parallel}}$ ,  $\Omega_{\text{drift}}$ , and  $\Omega_{\text{binormal}}$ , define the *streaming kernel*, hereafter referred to as  $\text{str}$ . The last term in Eq. 2 is a type of convolution (a Poisson bracket in real space). This defines the *nonlinear kernel* and is hereafter referred to as  $\text{n1}$ . Finally, note that explicit coupling with the Maxwell equations is also required to advance  $\tilde{\Psi}_a$  in time. This operation defines the *field solve* kernel, hereafter referred to as  $\text{field}$ .

### FFT-based evaluation of the nonlinearity

The treatment of the quadratic nonlinearity, through numerical evaluation of the convolution given in Eq. (2), is done in a standard way using a 2D Fast-Fourier transform (FFT) with dealiasing. The convolution can be evaluated by direct summation (and pruning unused wavenumbers), but to do so would be prohibitively slow for typical nonlinear simulations. Alternatively, one performs forward transform, multiplies the functions in real-space, following by the reverse transform. Uncorrelated, this procedure gives rise to aliasing. So instead we zero-pad the spectral representation by a factor of 3/2, take the forward transform to a finer real-space mesh, multiply, take the reverse transform, and retain only the original wavenumbers. The dealiased convolution conserves important flow invariants and eliminates a class of nonlinear instabilities from the numerical solution. First, we perform a series of four 2D complex-to-real (c2r) transforms

$$(\tilde{h}_a)_x \tilde{\Psi}_a \rightarrow \frac{\partial \tilde{h}_a}{\partial \xi}, \quad (\tilde{h}_a)_y \tilde{\Psi}_a \rightarrow \frac{\partial \tilde{h}_a}{\partial \xi} \quad (6)$$

$$(\tilde{h}_a)_x \tilde{\Psi}_a \rightarrow \frac{\partial \tilde{h}_a}{\partial \xi}, \quad (\tilde{h}_a)_y \tilde{\Psi}_a \rightarrow \frac{\partial \tilde{h}_a}{\partial \xi} \quad (6)$$

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