# GYRO: A 5-D gyrokinetic-Maxwell solver

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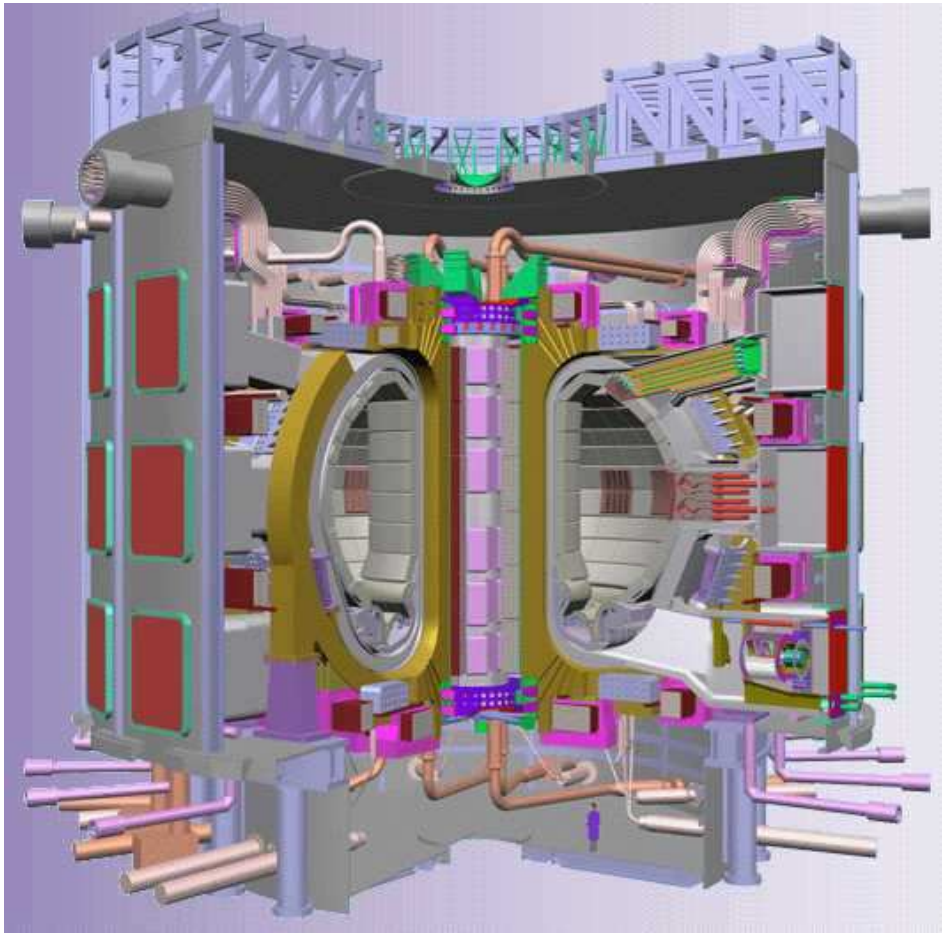
# Tokamak microturbulence and the GYRO code

- The most aggressively studied concept for **power production** by fusion reactions is the **tokamak**
- Uncertainties remain in predicting the **confinement** properties and performance of successively larger, **reactor-scale** devices
- **Turbulence** causes a **slow loss** of plasma to the tokamak wall, but confinement is still a factor of $10^5$ better than without a magnetic field



ITER: an experimental fusion reactor based on the **tokamak** concept

# Simulation of tokamak microturbulence

## Basic concepts and equations

- **Single-particle motion** in electromagnetic fields via Hamiltonian description:

$$H(x,p) = \frac{1}{2}(p - A)^2 + \phi(x)$$

- Ensemble of particles, $f(x,p,t)$, satisfies a **kinetic equation**

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + [f, H] = 0$$

- But $H$ depends on potentials $(\phi, A)$, which in turn depend on $f$,

$$\phi = \phi[f], \qquad A = A[f]$$

# Simulation of tokamak microturbulence (cont.)

## Average over gyromotion

- Particles exhibit fast gyromotion about a **gyrocenter**, $R$: $x = R + \rho(\vartheta)$
- Eliminate the timescale by **averaging over the gyroangle**, $\vartheta$
- The gyrokinetic-Maxwell (GKM) equations couple an averaged distribution $h$ to the electromagnetic fields $\Phi$:

$$\partial_t h = \mathcal{L}_a h + \mathcal{L}_b \Phi + \{h, \Phi\}$$

  - $\mathcal{F}\Phi = \int\int dv_1 dv_2\, h$ are the **Maxwell equations**
  - $\mathcal{L}_a$, $\mathcal{L}_b$, and $\mathcal{F}$ are **linear operators**
  - $f(r, v_1, v_2)$ is discretized over a 5-d grid (3 spatial, 2 velocity)
  - electromagnetic fields $\Phi(r) = [\phi, A_{||}]$ are **independent of velocity**
  - where $\phi$ and $A_{||}$ are the **electrostatic** and **electromagnetic** potentials

# Simulation of tokamak microturbulence (cont.)

## Specific Eulerian formulation

- $h = f + z v_{\|} A_{\|}$ and

$$\frac{\partial h}{\partial t} + \left( \frac{v_{\|}(\theta)}{qR} \frac{\partial}{\partial \theta} + i\omega_D \right) (h - \langle U \rangle) + i\omega_* \langle U \rangle + i\frac{q}{r}\{\langle U \rangle, h\} = 0$$

- the operator $\langle \cdot \rangle$ represents a **gyroaverage**
- $U = \phi - v_{\|} A_{\|}$
- $\omega_D$ is the **curvature drift operator**
- $\omega_*$ represents the **instability drive**

# GYRO overview

- **5-d Eulerian GKM solver** developed by Jeff Candy and Ron Waltz at General Atomics
- Computes the **turbulent radial transport** of **particles** and **energy** in tokamak plasmas
- Electron parallel motion treated implicitly, and other dynamics explicitly, using **Implicit-Explicit (IMEX) Runge-Kutta** time-integration scheme
  - Discretized on an **Eulerian grid** (not PIC).
- both **global** and **electromagnetic** capabilities
  - Radially global: able to accomodate arbitrary profile variation
  - Electromagnetic fluctuations with real electrons ($m_i/m_e = 3600$)
- Toroidally **spectral** (single-$n$ to full torus)
  - Can switch between global and flux-tube operational modes
- **Most comprehensive GKM code, worldwide**

# Discretization schemes

- **toroidal angle**: fully spectral
- **radius**: upwind differencing for linear advective derivatives on $f$, and centered differencing for field derivatives
- **poloidal angle**: upwind differencing for $\partial f/\partial\tau$, and centered differencing for $\tau$ field derivatives
- **velocity-space**: Gauss-Legendre quadrature for velocity-space integration
- **nonlinearity**: nonlinear Poisson bracket approximated with conservative difference-spectral analogue of the Arakawa method
- **collisions**: represented by second-order diffusive-type operator
- **time-advance**: second-order IMEX RK scheme for electron parallel motion

# GYRO accomplishments

## Comparison with DIII-D L-mode $\rho_*$ experiments

- calculations **matched experimental results** for electron and ion energy transport [1] within experimental error bounds
- **Bohm-scaled diffusivity** of the experiments was reproduced
- most physically comprehensive tokamak turbulence simulations ever undertaken

## Evaluation of minimum-$q$ theory of transport barrier formation

- found that a **minimum-$q$ surface** (where $s = 0$) in a tokamak plasma **does not** act as the catalyst for ion **transport barrier** formation [4]
- it was clearly shown that **transport is smooth** across an $s = 0$ surface due to the appearance of **gap modes**

# GYRO accomplishments

## Resolving the local limit of global GK simulations

- a global transport scaling study [6] overestimated the benchmarked local value [5], contradicting the **local hypothesis** which states that global and flux-tube simulations should agree at small $\rho_*$
- GYRO found an ion diffusivity $\chi_i$ that **matched the Cyclone value** at small $\rho_*$ [3]
- GYRO further showed for these large-volume simulations, there is a **long transient** period for which $\chi_i$ exceeds the statistical average

## Particle and impurity transport

- **first systematic gyrokinetic study** of particle transport, including impurity transport and isotope effects
- found that in a burning D-T plasma, the **tritium is better confined than deuterium**, with the implication that the D-T fuel will separate as tritium is retained

# GYRO performance: Two physical test problems

1. Waltz Standard Case Benchmark (WSCk)

2. Plasma Edge Case

**Problem size fixed in scaling study (strong scaling)**

# GYRO performance: Test platforms

1. **Cray X1 at ORNL:** 512 multistreaming processors
2. **AMD cluster at PPPL (Princeton):** 48 2-way Athlon MP2000+ (1.667 GHz), gigE interconnect
3. **IBM p690 cluster at ORNL:** 27 32-way p690 SMP nodes (1.3 GHz Power4), Federation Switch
4. **IBM Nighthawk II cluster at NERSC:** 416 16-way SMP nodes (375 MHz Power3), SP2 Switch
5. **SGI Altix at ORNL:** 256-way single-system image, NUMAflex fat-tree interconnect, 1.5 Ghz Itanium II

# GYRO performance – communication design

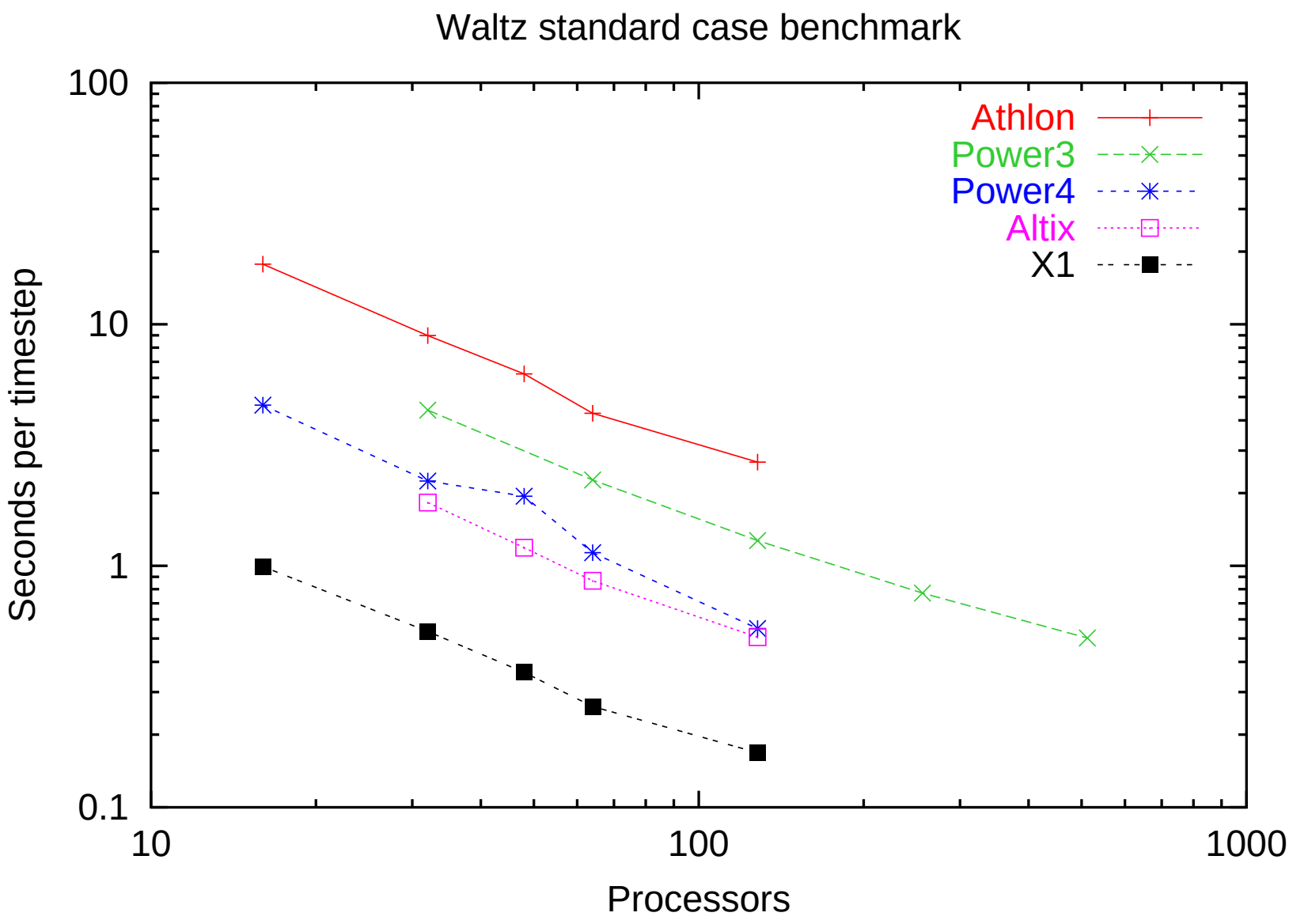
## Summary of message-passing design GYRO

- **Transpose operations** coded using loops over MPI_ALL_TO_ALL. Performance of these routines is the ultimate scaling limiter.
- Implementation details
  - created TRANSPOSE and SSUB libraries to perform 3-index row transposes and 2-index column tranposes,
  - utilizing subcommunicators COMM_ROW and COMM_COLL
- code has been run up to 2000 processors on Power3 cluster at NERSC (Seaborg), but scaling flattened out fairly quick after 512 processors

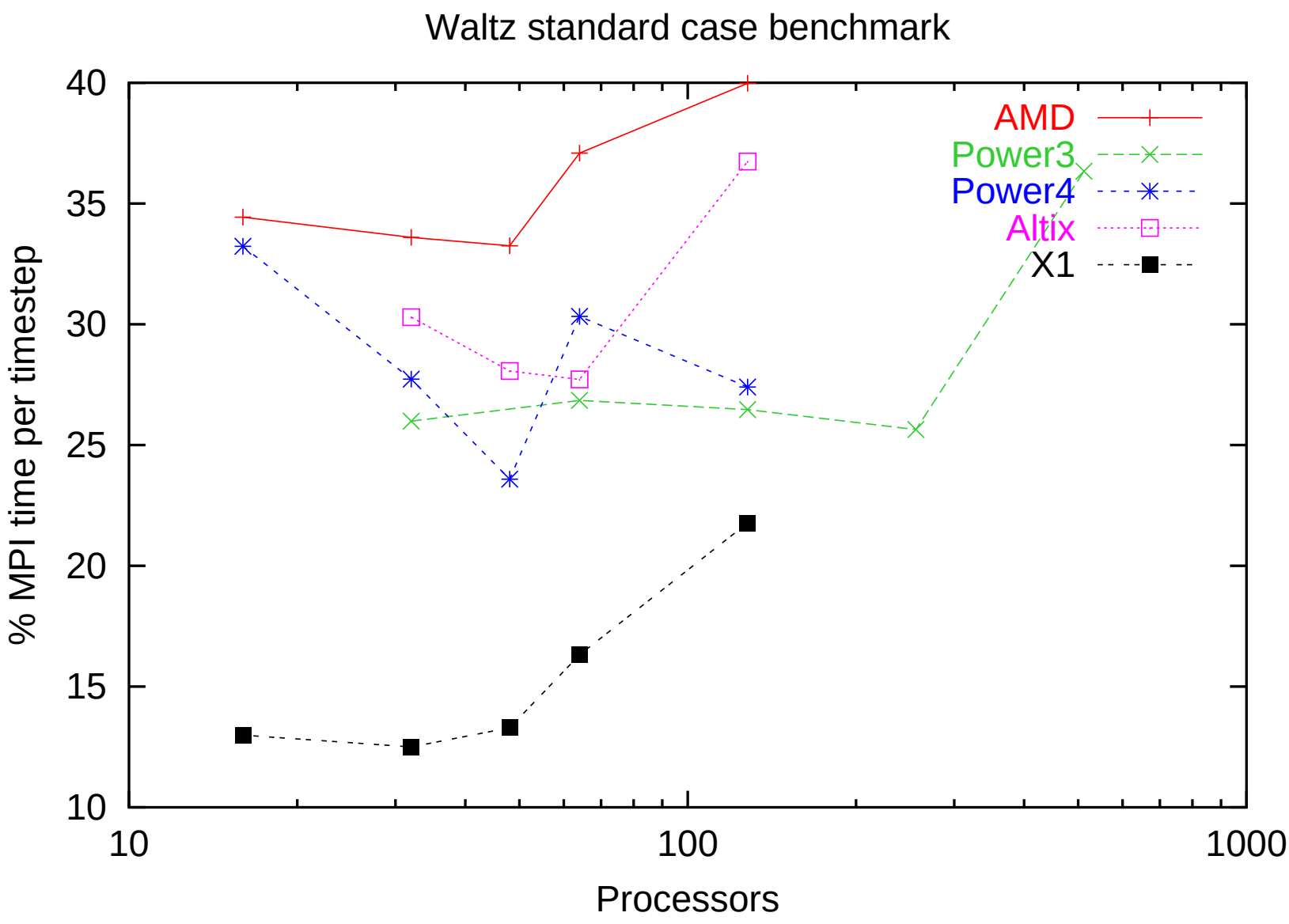
# GYRO performance – Waltz standard case

## Problem 1: Waltz Standard Case

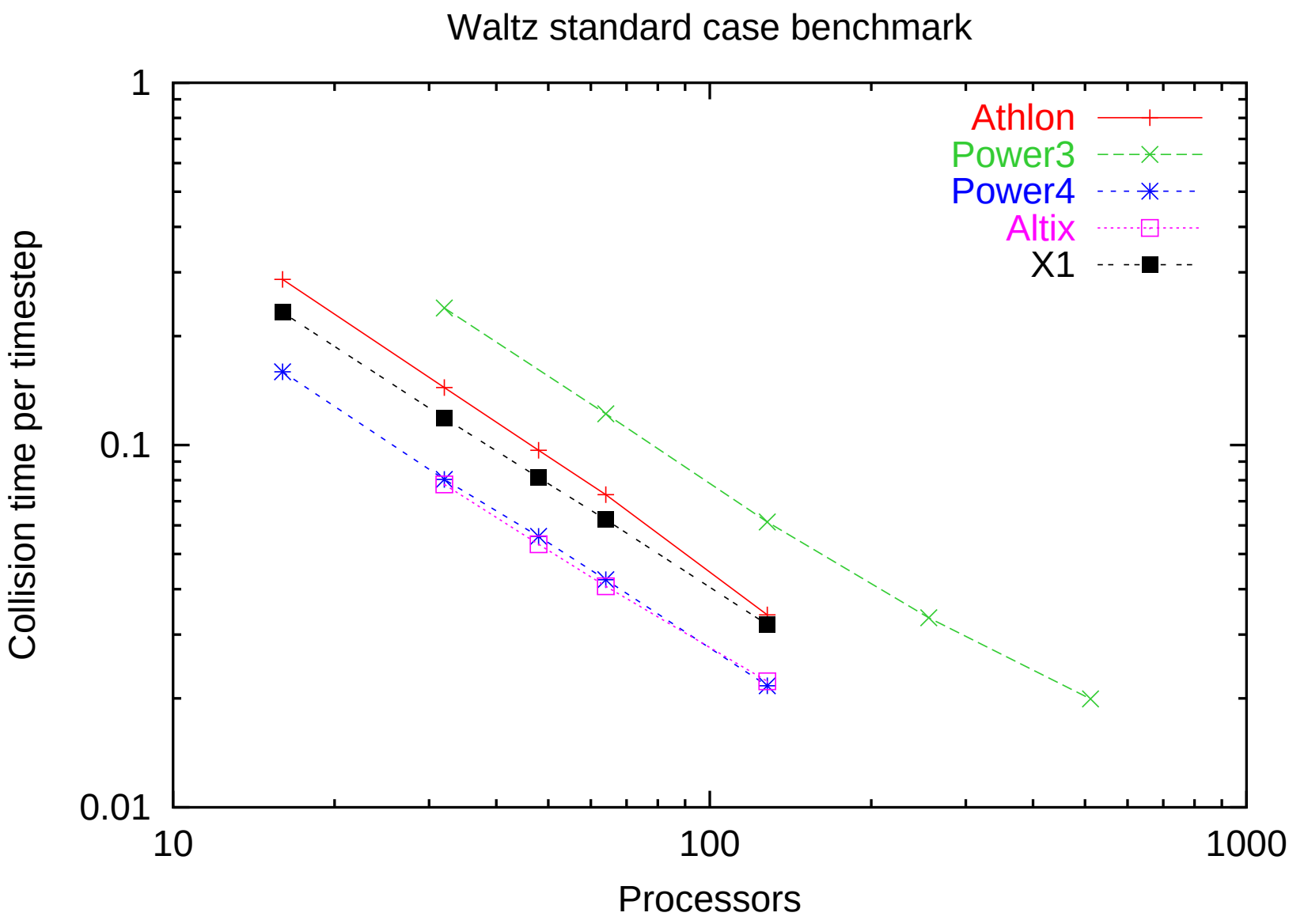
- parameters defined in [2], used as reference case in various publications
- no electromagnetic effects
- electron collisions
- flux-tube, 16 toroidal modes, electrons and ions
- $16 \times 140 \times 8 \times 8 \times 20 \times 2$ grid
- grid typical of production runs and represents roughly the minimum grid size to obtain physically accurate results
- grid is **relatively coarse**


Waltz standard case benchmark
Athlon
Power3
Power4
Altix
X1
Seconds per timestep
100
10
1
0.1
10
100
1000
Processors

Time/step




MPI Time/step

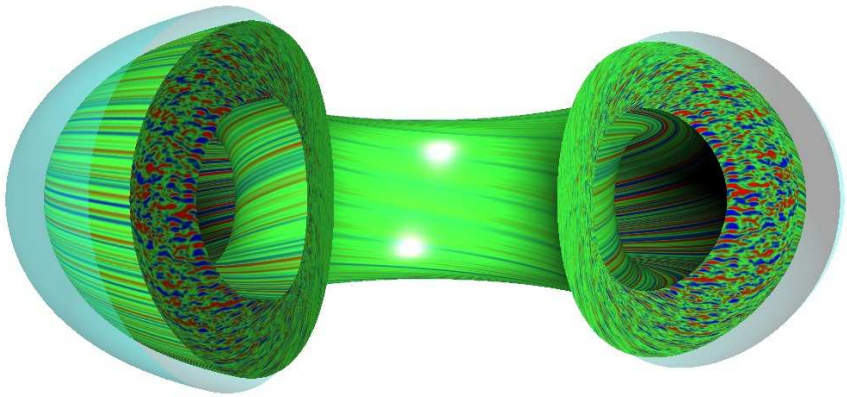



Collision time/step

# GYRO performance – Plasma edge case

**Problem 2: Plasma edge case**

- prototype case to explore parameter space characteristic of the plasma edge
- magnetic shear and safety factor are high at the outer plasma boundary, and equilibrium gradients are steep
- global, 28 toroidal modes, ions only (adiabatic electrons)
- $28 \times 200 \times 10 \times 10 \times 28 \times 1$ grid



Time in milliseconds

| Machine | processors | time/step | %MPI-time/step | Steps/sec |
|---|---|---|---|---|
| IBM Power3 cluster | 896 | 602.45 | 17.2 | |
| | 1344 | 544.58 | 14.9 | |
| | 1792 | 405.19 | 16.7 | 2.5 |
| | 2240 | 431.48 | 17.0 | |
| | 2688 | 422.91 | 15.7 | |
| IBM Power4 cluster | 224 | 994.94 | 21.1 | |
| | 448 | 561.21 | 23.9 | 1.8 |
| SGI Altix | 224 | 554.12 | 34.0 | 1.8 |
| Cray X1 | 224 | 121.98 | 12.3 | |
| | 448 | 72.25 | 9.6 | |
| | 504 | 62.35 | 9.7 | 16 |

# Conclusions

- GYRO development has reached all its **original capability objectives**
- Refinements are continually being added
- Several important research results have been obtained just over the last year and a half
- X1 has provided a platform where **new physics scenarios** have been **quickly designed and analyzed** just in the last year
- The performance of GYRO on nonvector machines is constrained by communication bandwidth; not true on X1, where the GYRO MPI_ALL_TO_ALL costs have dropped to the lowest levels ever
- Collisions perform rather poorly on the X1 despite several optimizations to improve vectorization to its current state. Any further improvement will probably be gained via a new algorithm.

# References

[1] J. Candy and R.E. Waltz. Anomalous transport in the DIII-D tokamak matched by supercomputer simulation. *Phys. Rev. Lett.*, 91:045001–1, 2003.

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[4] J. Candy, R.E. Waltz, and M.N. Rosenbluth. Smoothness of turbulent transport across a minimum-$q$ surface. *Phys. Plasmas*, 11:1879, 2004.

[5] A.M. Dimits, G. Bateman, M.A. Beer, B.I. Cohen, W. Dorland, G.W. Hammett, C. Kim, J.E. Kinsey, M. Kotschenreuther, A.H. Kritz, L.L. Lao, J. Mandrekas, W.M. Nevins, S.E. Parker, A.J. Redd, D.E. Shumaker, R. Sydora, and J. Weiland. Comparisons and physics basis of tokamak transport models and turbulence simulations. *Phys. Plasmas*, 7:969, 2000.

[6] Z. Lin, S. Ethier, T.S. Hahm, and W.M. Tang. Size scaling of turbulent transport in magnetically confi ned plasmas. *Phys. Rev. Lett.*, 88:195004, 2002.