New Developments and Future Directions for M3D-C1

Nate Ferraro

Princeton Plasma Physics Laboratory

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Applications of M3D-C1 Focus on Stability, 3D Equilibria, and Disruptions

- **Stability**
  - Classical tearing stability; locked modes
  - EHO stability in QH-mode discharges
  - Effect of pellet injection and pedestal structure on ELM stability

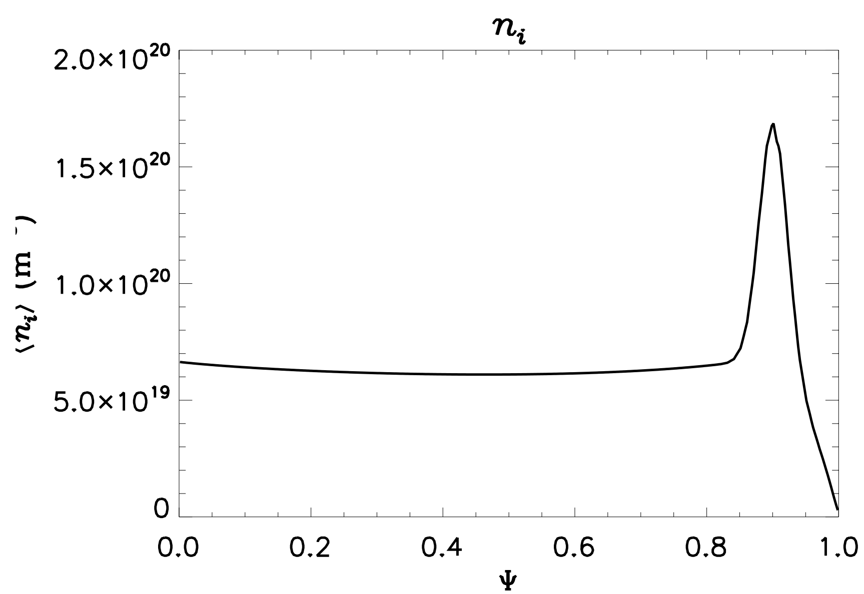
- **3D Equilibria**
  - Plasma response in ELM-mitigation experiments (Lyons)

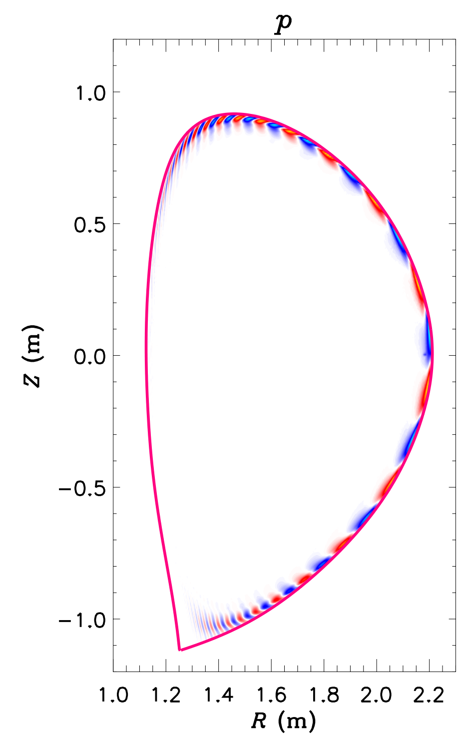
- **Disruptions**
  - Nonlinear evolution of VDEs (Pfefferlé) and tearing modes

New Pellet Modeling Capabilities Are Being Applied to ELM Stability

- **Parks model of pellet ablation implemented by Alex Fil (PPPL)**

- **Effect of density "bumps" on ELM stability explored by Steffi Diem (ORNL)**





Ongoing & Future Development Emphasizes Integrated Modeling and Disruptions

- **Coupling with gyrokinetic codes (XGC, GTC) for calculating transport in 3D geometry**
  - Goal is to understand how transport due to 3D fields affects pedestal structure
- **Implementation of self-consistent fast ion species (Breslau)**
- **Integration with edge codes & improved edge modeling**
  - Neutrals, radiation
- **Disruptions are a primary focus**
  - VDE calculations are being done to predict wall forces in NSTX-U and guide diagnostics development (Pfefferle)
  - M3D-C1 calculations are being used as a basis for RE modeling (Hirvijoki)
  - How do instabilities lead to disruptions?

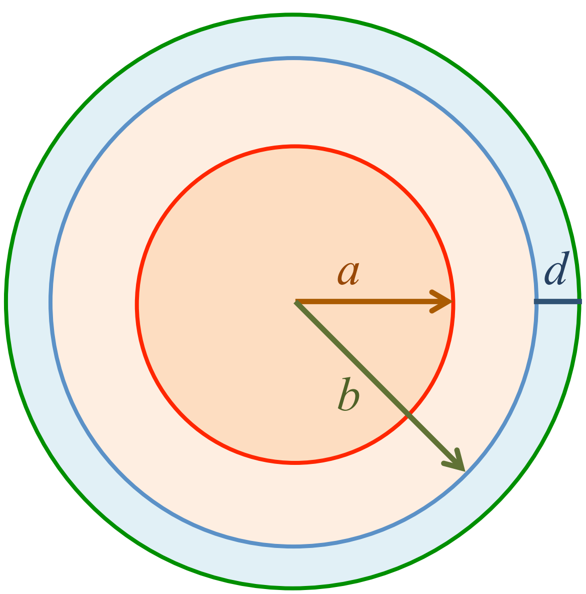
Resistive Wall Modes

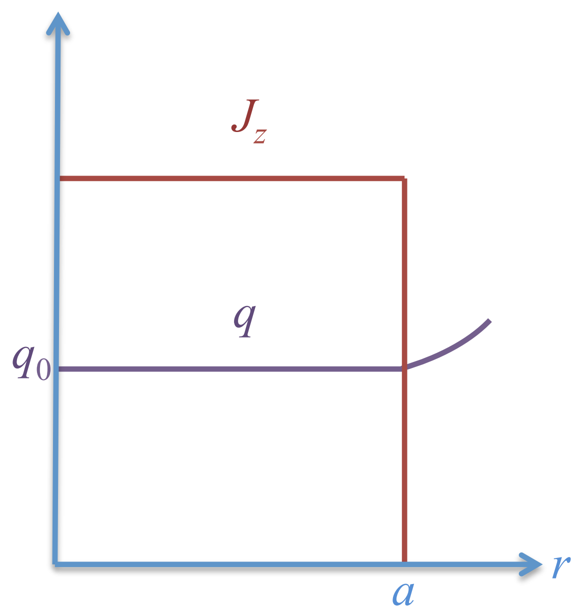
RWMs in Shafranov Equilibrium Have Analytic Solution for Code Verification

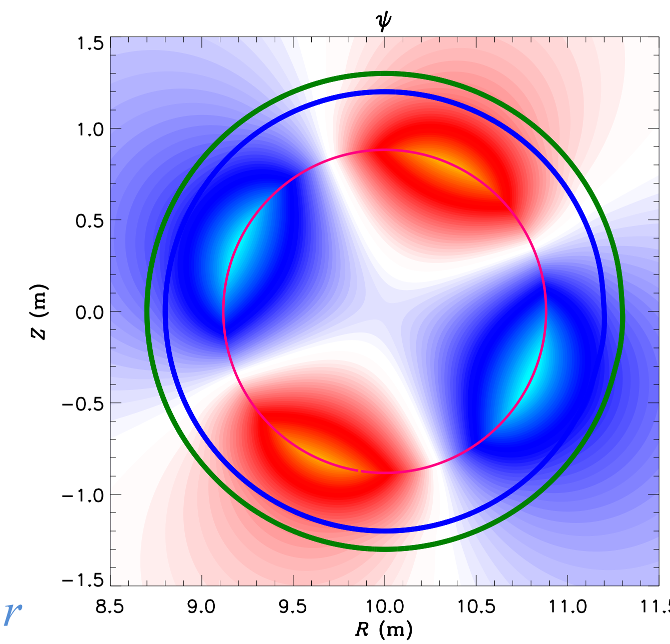
- **Circular cross-section, cylindrical plasma with constant q, current density (J_z) and mass density (ρ_0) (Shafranov equilibrium)**

- **Analytic thin-wall solution provided by Liu *et al.* *Phys. Plasmas* 15, 072516 (2008)**

Wall time: $\tau_W = \mu_0 bd/(2\eta_W)$
Alfven time: $\tau_A = (\mu_0 \varrho_0)^{1/2} R_0/B_0$



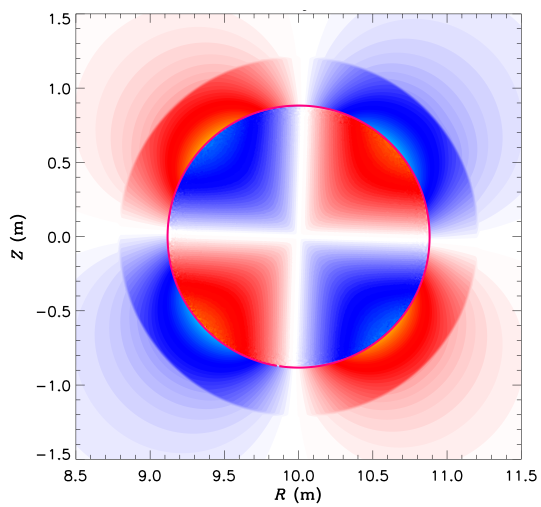


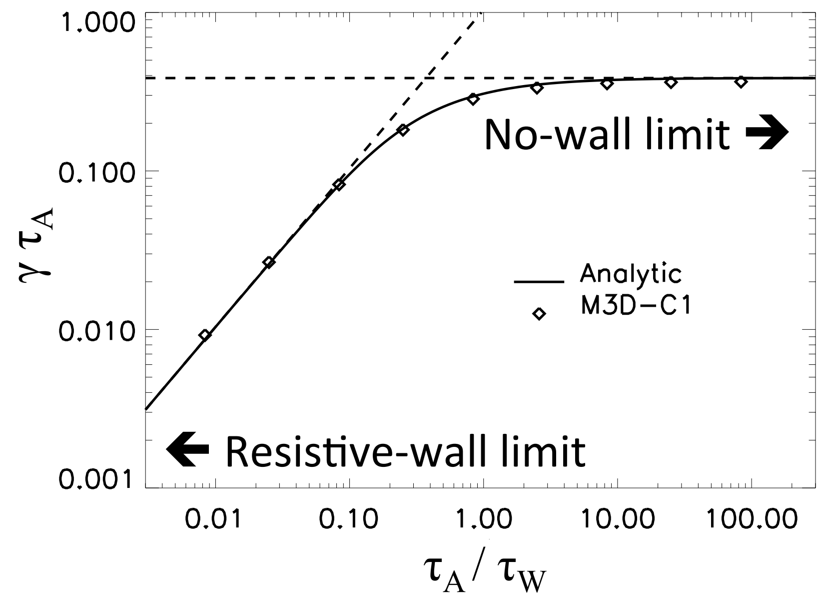


M3D-C1 Reproduces Analytic RWM Result in Thin Wall Limit

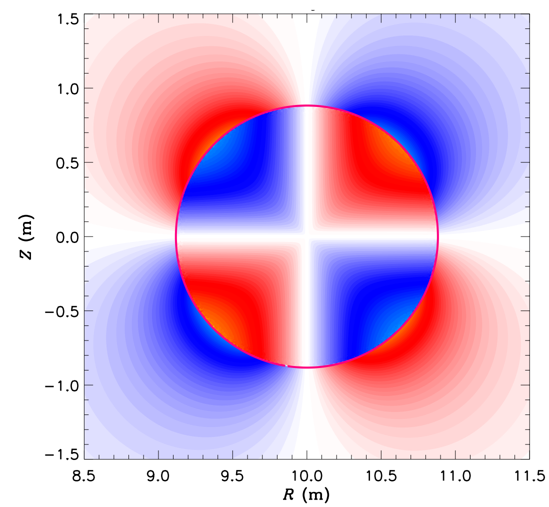
- **Growth rate calculated using linear, time-dependent calculation**
- **M3D-C1 agrees with analytic growth rate in both resistive-wall ($\tau_A << \tau_W$) and no-wall ($\tau_W << \tau_A$) limits**

Resistive-Wall Limit
B_θ Eigenfunction





No-Wall Limit
B_θ Eigenfunction

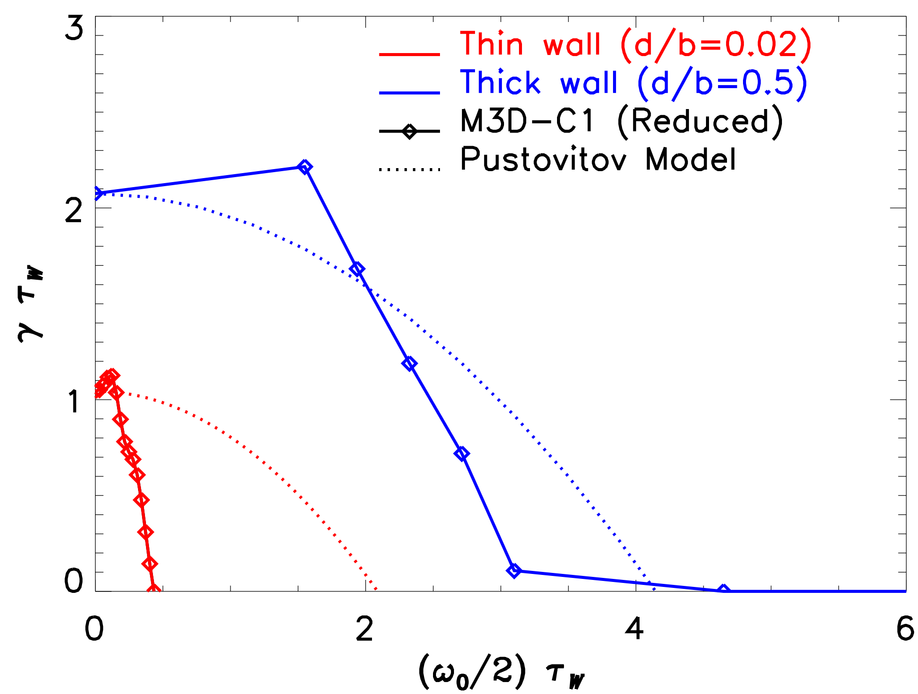


Complete Rotational Stabilization of RWM Observed

- **Reduced-model (2-field) calculations show stabilization of RWM by toroidal rotation**
  - $\omega = \omega_0 (1 - \psi_N)$

- **Qualitative agreement with Pustovitov model***
  - $\gamma = \gamma_0 [1 - (\omega/\omega_c)^2]$ where γ_0 is the growth rate with no rotation and $\omega_c = 2\gamma_0/n$
  - Pustovitov model derived in thick wall limit with uniform rotation

- **Need to revisit calculations to determine mode frequency vs. plasma rotation**



*Pustovitov *Nucl. Fusion* **53** (2013) 033001

Wesson Equilibrium has Smooth Profiles; Amenable to Solution with Full Model

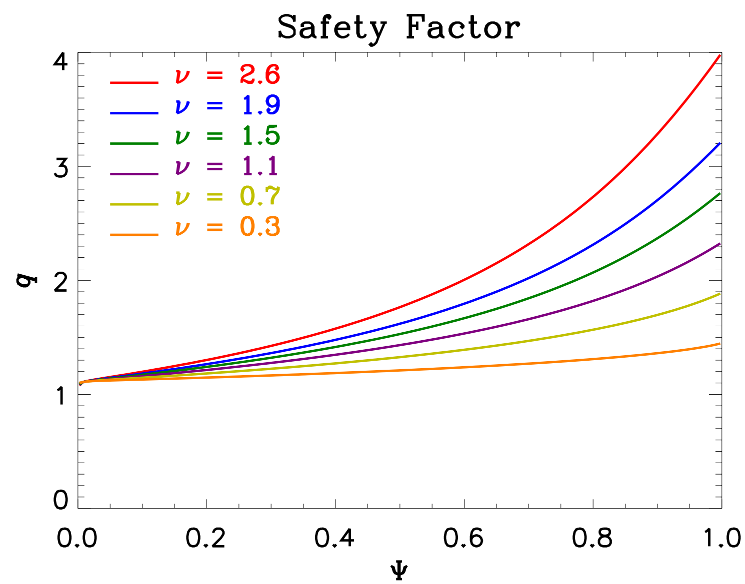
$$J_z = J_{z0}\left(1-\frac{r^2}{a^2}\right)^{\nu}$$

$$q_0 = \frac{2B_{z0}}{\mu_0 J_{z0} R_0}$$

$$q = q_0 \frac{r^2/a^2}{1-\left(1-\frac{r^2}{a^2}\right)^{1+\nu}}$$

$$R_0 = 10\,\mathrm{m}$$

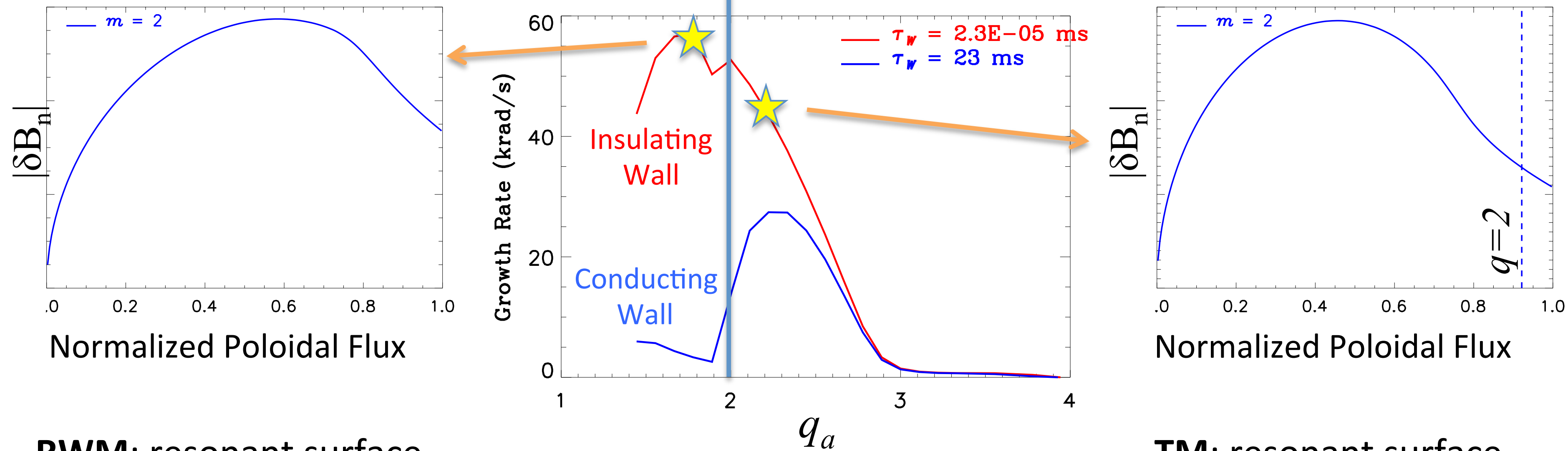
$$B_{z0} = 1\,\mathrm{T}$$



- **Fully compressible, resistive single-fluid MHD model**
- **$S_0 \approx 10^6$; Viscosity, thermal conductivity ≈ 0.2 m^2/s**
- **Scan q_a while holding $q_0 = 1.1$ constant**

Resistive Wall Modes and Wall-Stabilized Tearing Modes are Found

Resistive Wall Mode ← → Wall-Stabilized Tearing Mode



RWM: resonant surface (q=2) is outside plasma

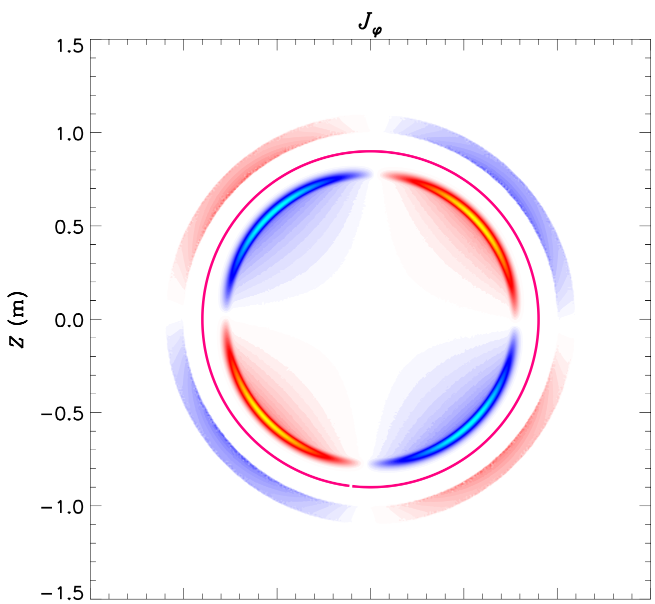
TM: resonant surface (q=2) is inside plasma

- **Transition between two modes is smooth because resistivity across limiting surface is smooth**

Current Density in RWM Eigenmode Peaks Where $\eta \approx \eta_W$

- **In RWM eigenmode, current density peaks at the "edge" of the plasma**
  - The "edge" is defined by the resistivity profile

$$\eta = \eta_0 + \frac{1}{2}\eta_{vac}\left(1 + \tanh\left[(\Psi - 1)/\Delta\Psi\right]\right)$$



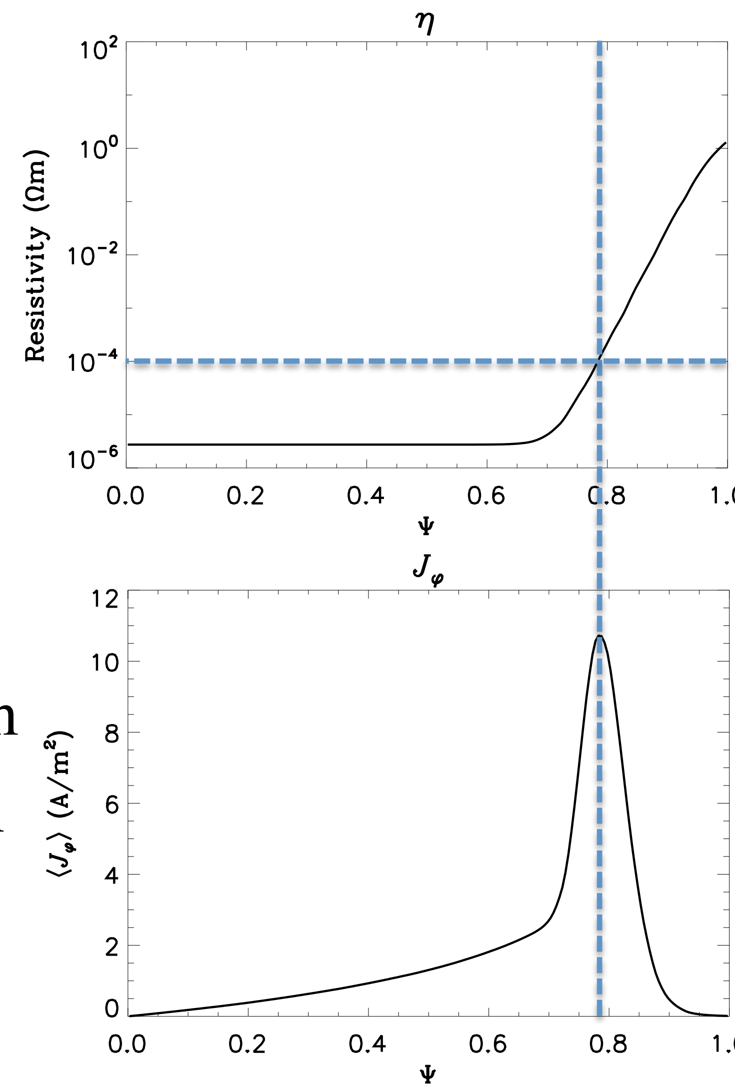
$$\eta_{vac} = 2.74\ \Omega\mathrm{m}$$

$$\eta_W = 2.74\times10^{-4}\ \Omega\mathrm{m}$$

$$\eta_0 = 2.74\times10^{-6}\ \Omega\mathrm{m}$$

$$\Delta\Psi = 0.04$$

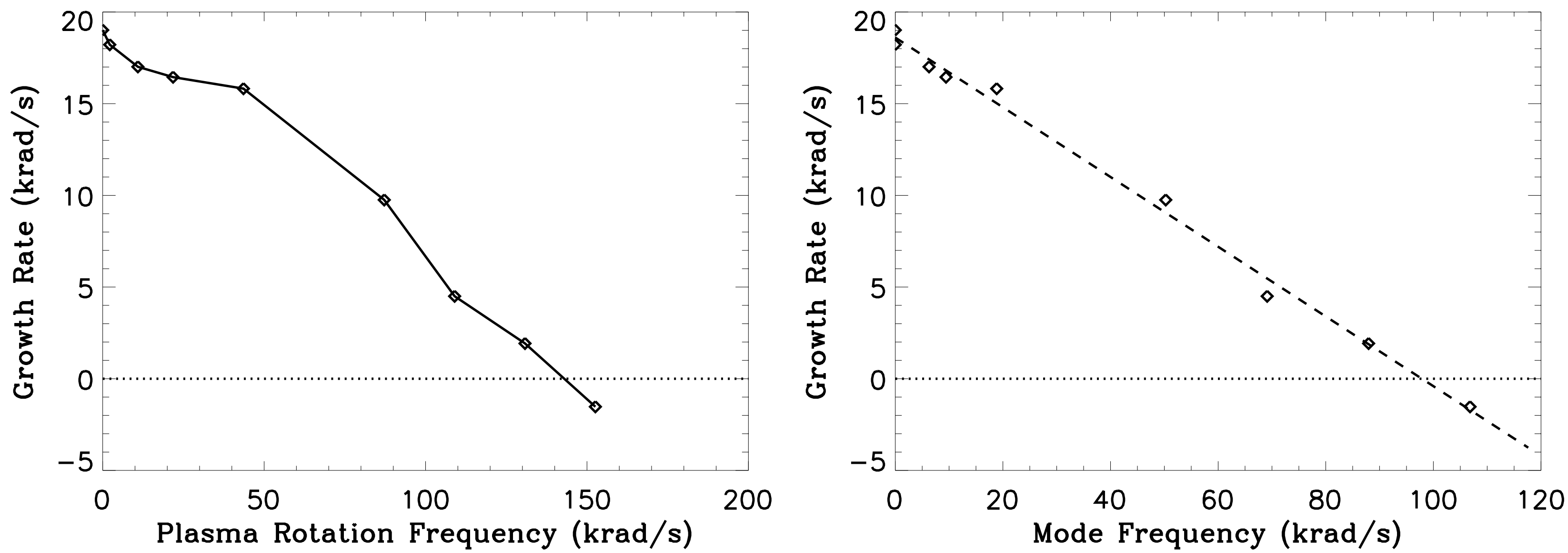
$$q_a = 1.8$$



RWM is Completely Stabilized by Rotation

- **Uniform toroidal rotation is considered**

$q_a = 1.8$ $\tau_W = 0.23$ ms $2\pi/\tau_W = 27$ krad/s

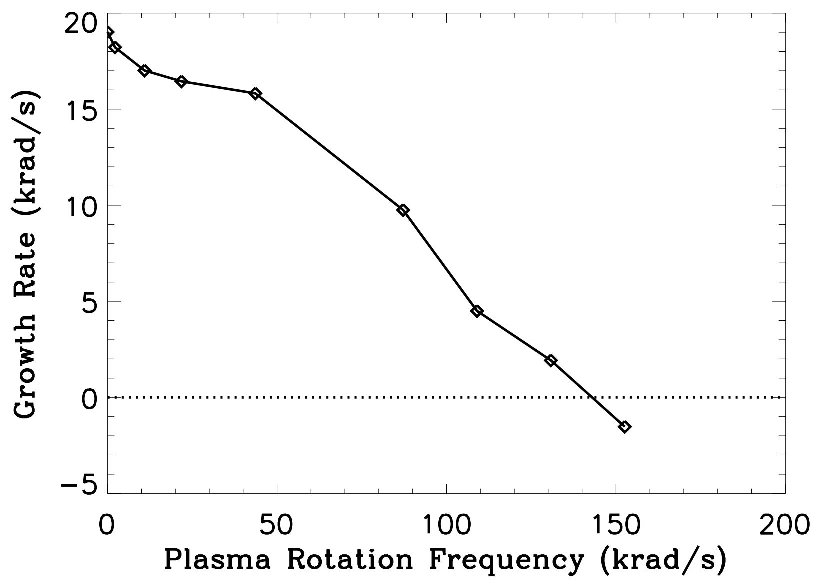


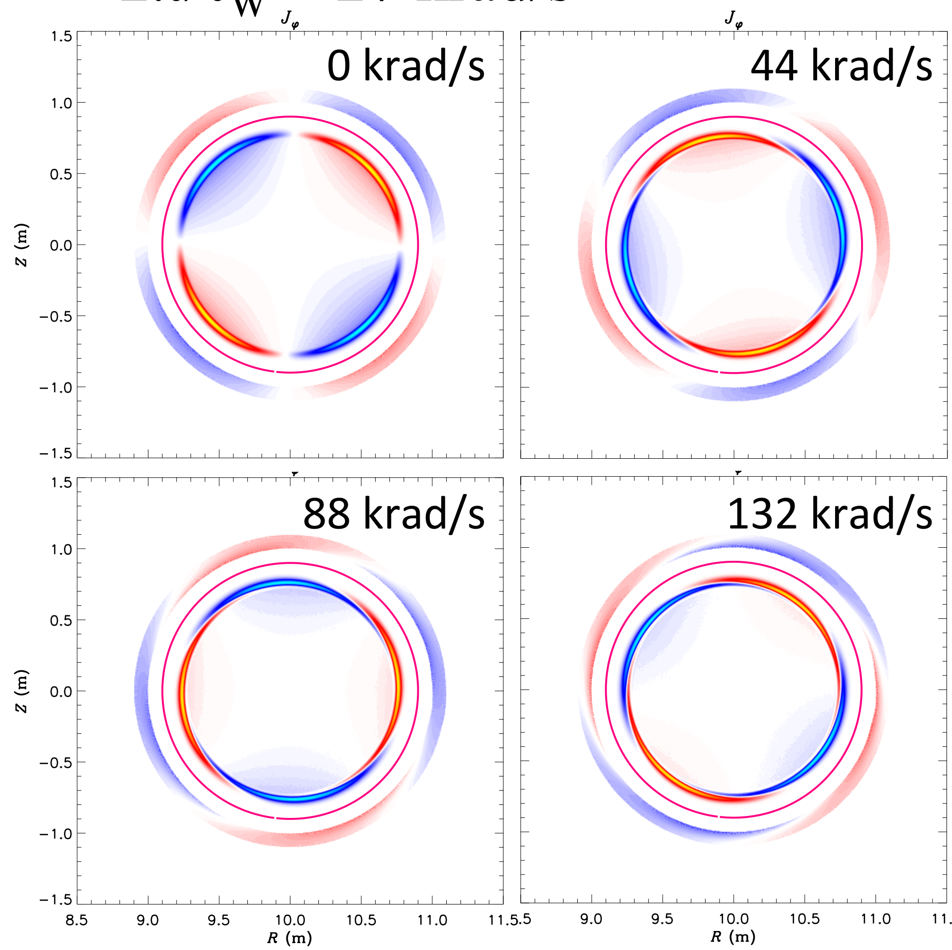
- RWM growth rate appears to be linear function of mode frequency
  – Complete stabilization is found when $\omega_{RWM}\tau_W \sim 25$

RWM Eigenmode is Sheared by Rotation

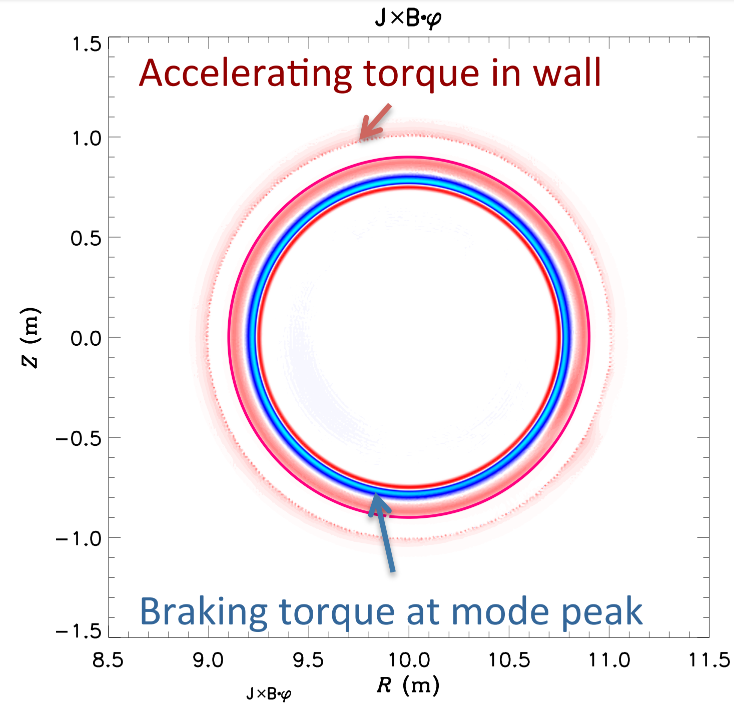
- **Uniform toroidal rotation is considered**

$q_a = 1.8$ $\tau_W = 0.23$ ms $2\pi/\tau_W = 27$ krad/s

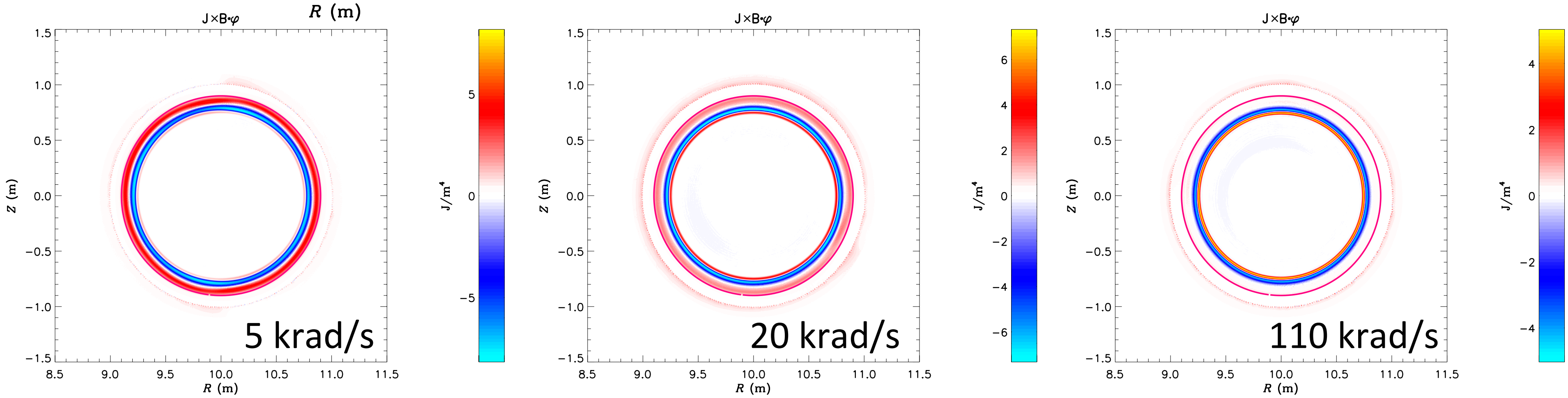




Quasilinear Torque is Maximum When $\omega_{RWM} \sim 2\pi/\tau_W$



- **Net quasilinear torque on plasma always opposes mode rotation**
  - Equal and opposite to torque on wall
- **Torque deposition inside plasma changes with ω_{RWM}**
  - Braking near peak of current density
  - Low ω_{RWM}: Acceleration outside mode peak
  - High ω_{RWM}: Acceleration inside mode peak

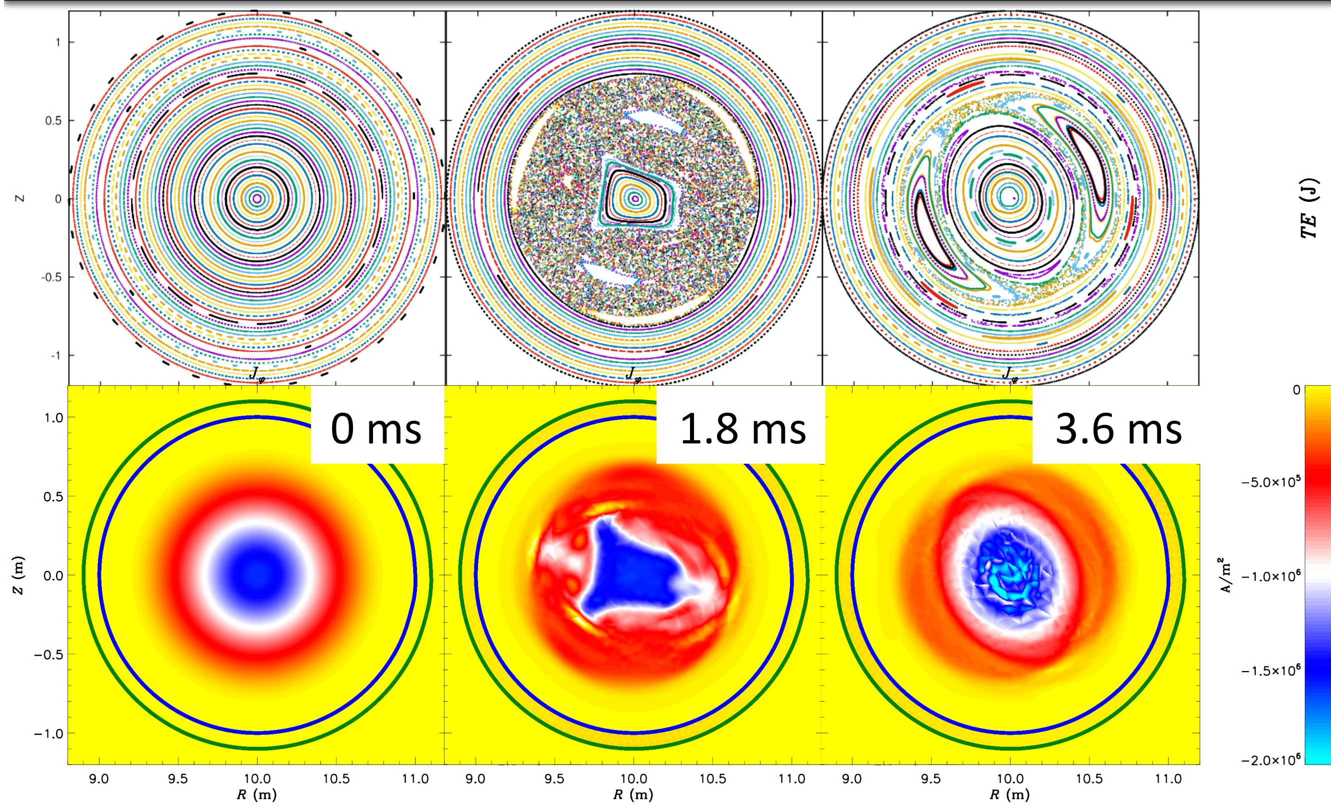


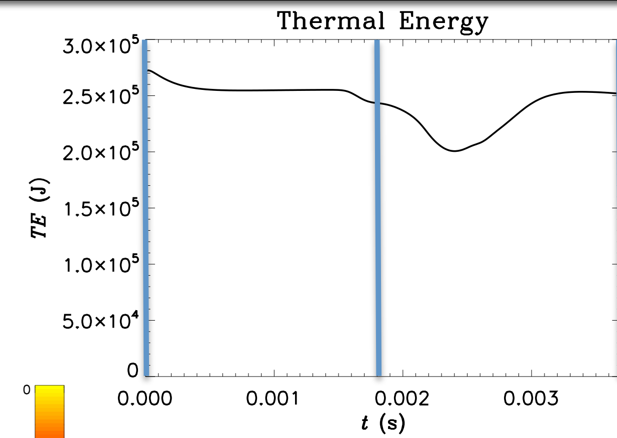
Ultimate Goal is to Address Disruption Physics

- **VDE calculations (David Pfefferlé)**
  - Demonstrated capability to simulate resistive timescales
  - Quantitative agreement with Halo current measurements

- **Nonlinear calculations of RWMs, Tearing Modes, and Locked Modes are being considered**
  - How do these instabilities lead to disruptions?
  - Nonlinear M3D-C1 calculations of these instabilities tend to show mode saturation, not disruption
  - Need more physics? Radiation / impurity transport?
  - Need More realistic equilibria that are less "passively stable"?

Nonlinear Modeling of Tearing Modes Shows Recovery to 3D Equilibrium





- **Loop voltage is applied to maintain current and provide heating**
- **TM fully stochasticizes plasma, but plasma recovers!**
  - Open field line region is never stochasticized, despite resistive wall
- **Effort is underway to model disruptions via radiative islands (Teng)**

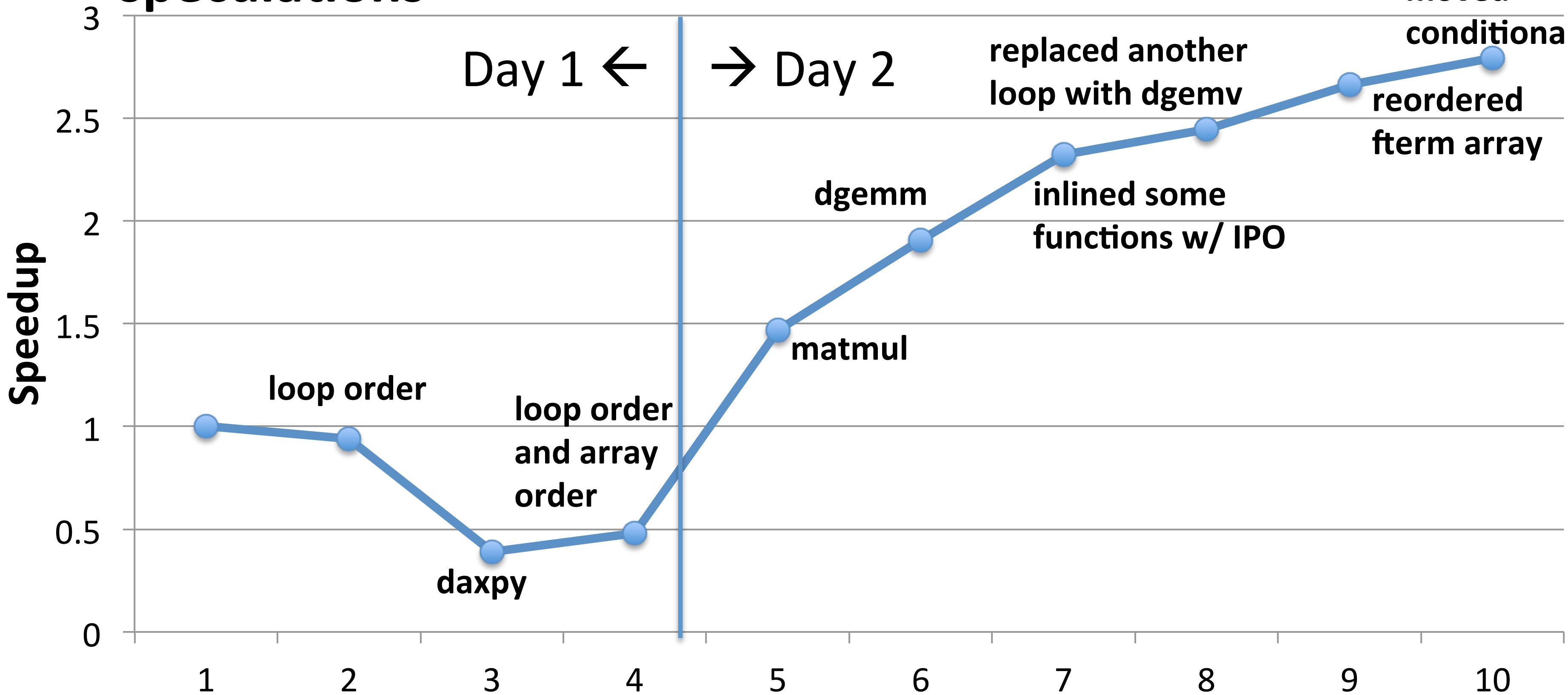
Optimization of M3D-C1 for HPC

M3D-C1 Kernel was Optimized for KNL at NESAP "Dungeon Session"

- **NESAP = NERSC Exascale Science Applications Program**
  - Collaboration between NERSC, Cray, Intel, and physics applications groups to optimize codes for KNL
- **KNL = Intel's "Knight's Landing" compute nodes**
  - Will be used on Cori Phase II
  - 68 cores / node
  - 94 GB DDR4 memory (on Cori II), peak bandwidth 100 GB/s
  - 16 GB MCDRAM / node, peak bandwidth 460 GB/s
- **We optimized two M3D-C1 kernels at "Dungeon Session" at Intel in August**
  - Matrix assembly kernel (not including communications)
  - PIC particle pushing kernel

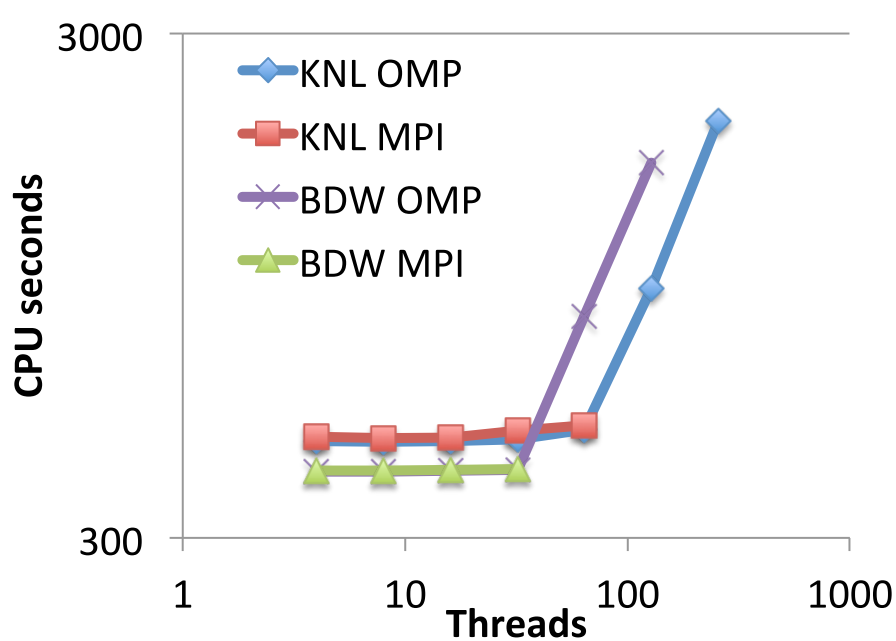
2.8x Speedup Achieved for Matrix Assembly Kernel on KNL

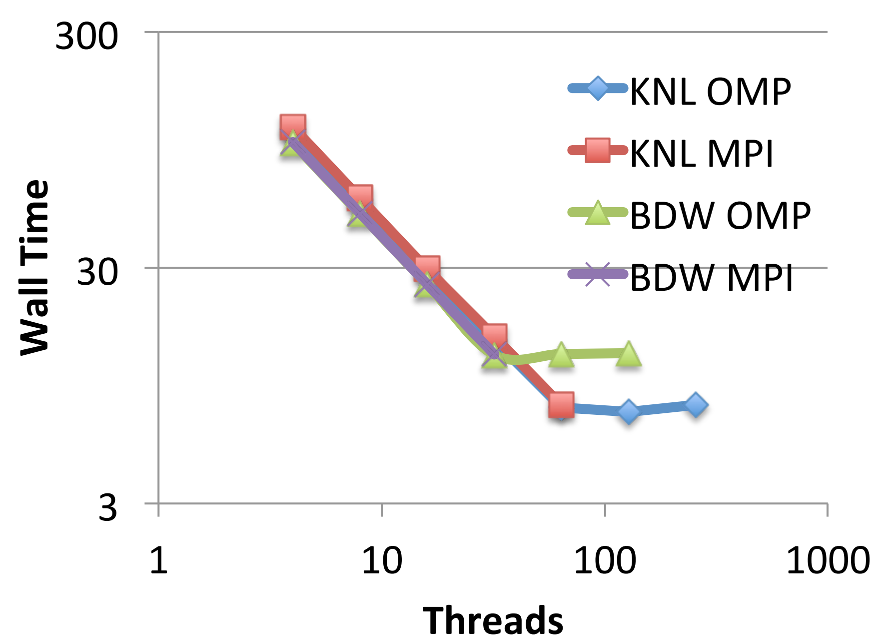
- **Replaced loops with level 2 & 3 BLAS**
- **Forced inlining of some functions w/ IPO**
- **Moved conditional outside loop to eliminate bad speculations**



Optimized Kernel Shows Improved Performance on KNL node vs. BDW

- **OpenMP and MPI scaling both nearly perfect up to 1 thread/core**
- **No speedup from multiple OMP thread/core**
  - Threads use full L2 cache
- **BDW is 15% faster per core, but KNL is 40% faster per node**





Conclusions from KNL Optimization Exercise

- **Don't try to outsmart compiler**
  - Manually changing loop order, data alignment, etc. never improved things
  - Architecture-specific optimizations will make code messy and won't be portable
- **Inlining helps compiler optimize loops**
  - Enable IPO when functions are in separate Fortran source file
- **Use Intel MKL BLAS as much as possible**
  - These are very well optimized for KNL
  - BLAS calls will be portable to other architectures
- **Optimizing full code will require optimized sparse solvers**

Upcoming Opportunities Will Require More Than Code Optimization

- **Upcoming SciDAC calls will have increased emphasis on HPC**
- **How can we take advantage of future HPC systems?**
  - PDE solves won't scale well
  - Ensemble runs (parameters scans, UQ) will be useful, but probably discouraged
- **"Multiphysics" is probably the answer**
  - Calculations of kinetic closures
  - Detailed local physics (e.g. atomic physics)
  - "Whole-device" modeling
- **Challenge: WDM only makes sense when components are coupled; yet coupling makes scaling difficult**

M3D-C1 at APS

- **ELM Pellet pacing**
  - Pellet ablation models and nonlinear evolution of kinetic profiles (Fil PP10.64)
  - Linear ELM stability in presence of density perturbations (Diem PP10.65)

- **Perturbed equilibrium calculations**
  - Toroidally localized turbulence from perturbed pressure profiles (Wilcox CO4.13)
  - Perturbed equilibria in RMP ELM-mitigated discharges (Lyons GP10.85; Park JO9.7)
  - Transport in RMP ELM-mitigated discharges (Callen PP10.70; Hager PP10.61)
  - Plasma response in snowflake geometry (Canal NP10.30)
  - Error field correction (Myers GO6.2) and penetration (Beidler GP10.76)
  - Effect of RMPs on divertor geometry (Shafer PP10.62)

- **Nonlinear evolution**
  - Sawtoothing / Hybrid-like plasmas (Krebs GP10.87)
  - Tearing modes (Teng GP10.79)