Highlights of recent work:

1. Effects of shaping on the Dimits nonlinear shift

   with Emily Belli

2. Implementation of equilibrium sheared flows in GS2

   with Bill Dorland & Nuno Loureiro

3. Algorithm studies

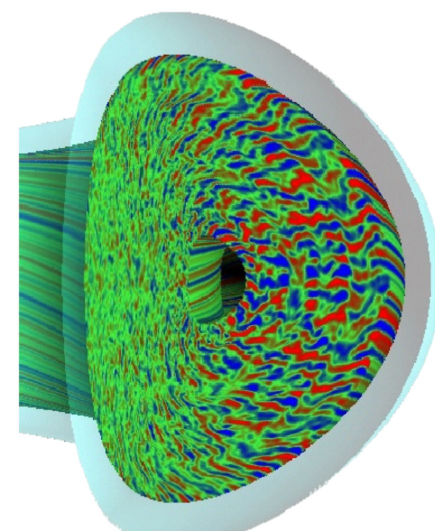
   (improved GMRES, Krylov solvers, TVD/CWENO shock-capturing algorithms, semi-implicit methods)

   (interactions with Jin Chen, Steve Jardin, Ravi Samtaney, David Keyes, Mark Adams, Jim Stone, Prateek Sharma, Nuno Loureiro, Eitan Tadmor)

Greg Hammett

PPPL theory microseminar 11/16/2006

(I only showed about half these slides for a ~10 min talk.)

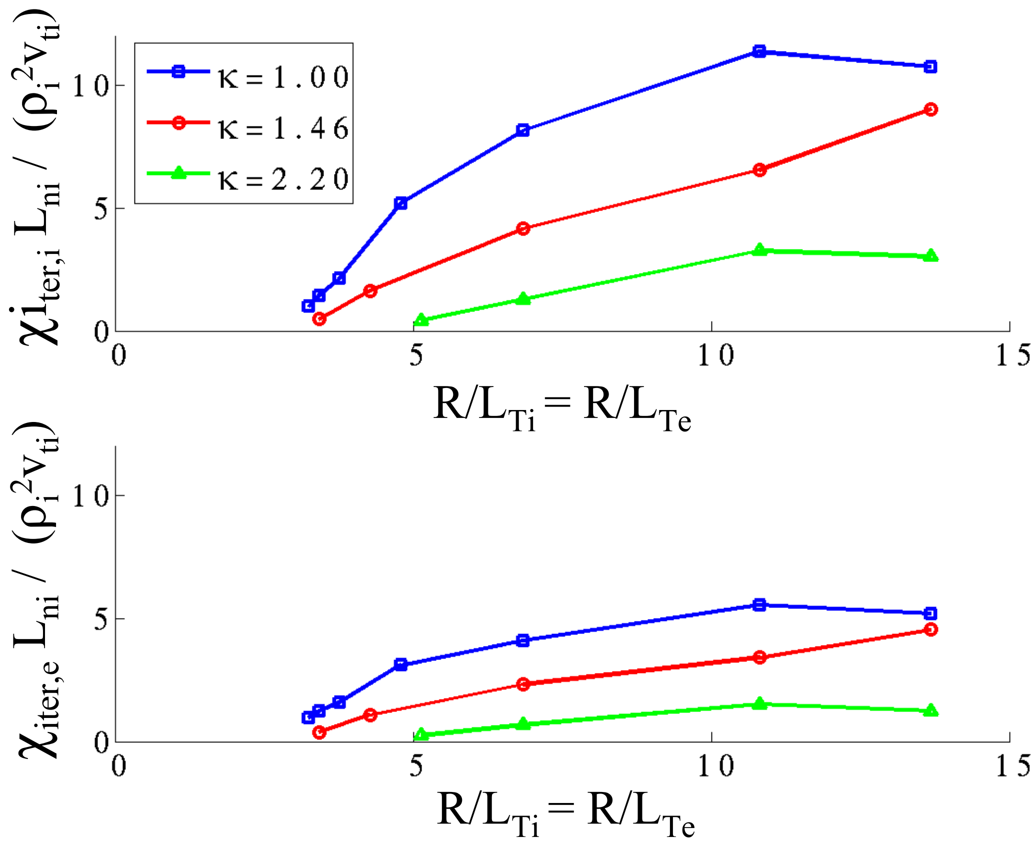


Candy & Waltz, General Atomics

Unlike the linear results, the nonlinear critical temperature gradient increases with strong shaping.

Nonlinear ion and electron heat fluxes vs. R/L_T

(Electrostatic)



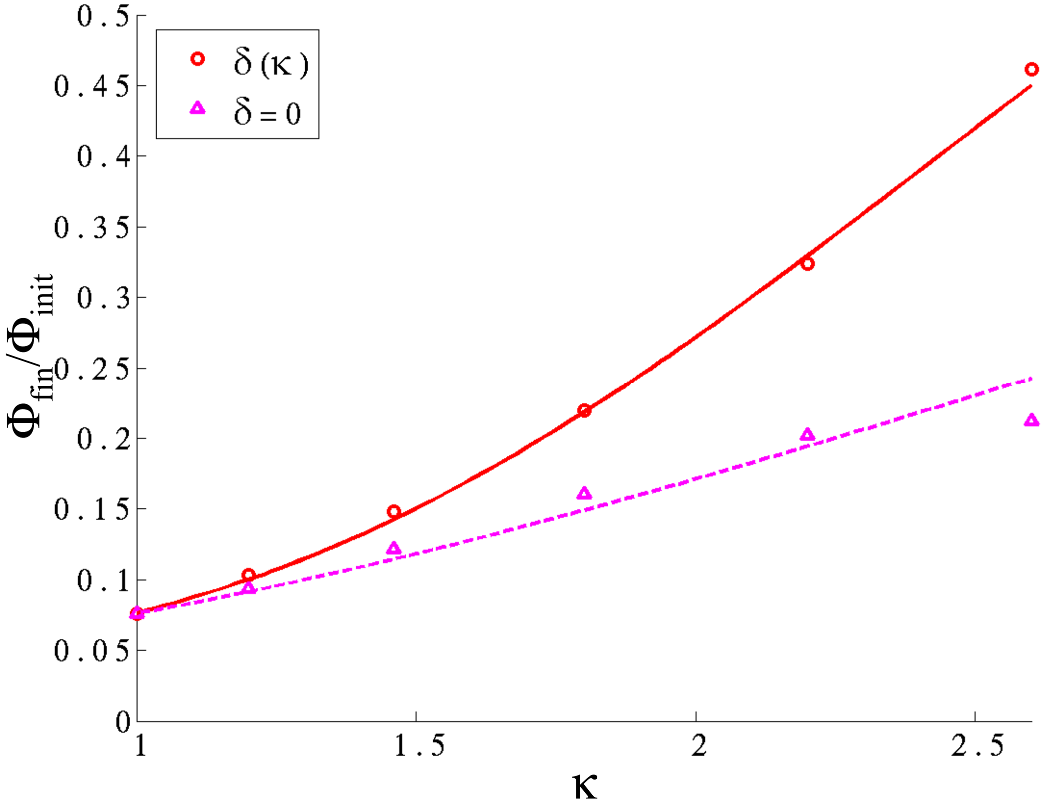
($\partial_\rho \beta$ is varied with κ & R/L_T)

Belli, Ph.D. Thesis 2006

The larger upshift of the nonlinear critical gradient with higher shaping may be due to enhanced zonal flows.

Amplitude of R-H residual zonal flows vs. κ

(data points are the GS2 results;
the lines are the analytic model prediction)



Overall, the geometry of residual zonal flows is important and may help explain why strong shaping is favorable in experiments.

A model prediction for the scaling of the R-H* h with shaping was found empirically based on the GS2 data. We assume:

$$\boxed{\frac{\Phi_{fin}}{\Phi_{init}} = \left(1 + \frac{1.6C}{h_{shaping}}\right)^{-1}}$$

where

$$h_{shaping} = \underbrace{\frac{\varepsilon^{1/2}}{q^2}}_{\text{Rosenbluth Hinton}} \underbrace{f(\kappa,\delta)}_{\text{shaping effects}}$$

(C=0.887 to match GS2 circular case (κ=1) with original R-H model.)

We found a good fit with:

$$\boxed{f(\kappa,\delta) = \tfrac{1}{2}\left[1 + \kappa^2\left(1 + r\frac{\partial\delta}{\partial r}\right)^2\right]}$$

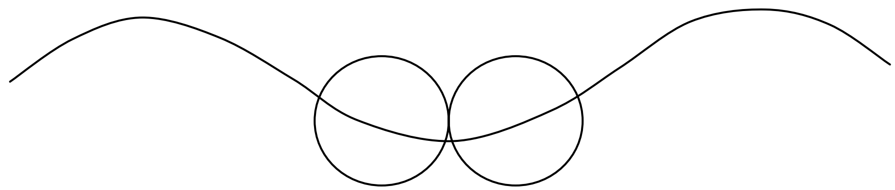
Analytic confirmation: Yong Xiao & Catto '06

* M. Rosenbluth & F. Hinton, Phys. Rev. Lett. **80**, 724 (1998).

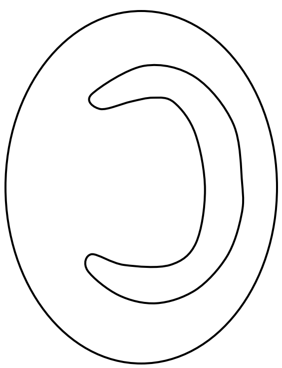
Physical picture of Hinton-Rosenbluth residual flow:

Classical polarization density:

$$n_{i,pol} = -\int d^3 \upsilon\, F_{M0} \frac{e}{T_i}\left(\Phi - \left\langle \left\langle \Phi \right\rangle_{gyroaverage} \right\rangle_{gc\_to\_particle} \right) = -n_{i0} k_\perp^2 \rho_i^2 \frac{e\Phi}{T_i}$$



Neoclassical polarization density (enhanced by larger banana widths):



$$n_{i,pol} = -n_{i0} \underbrace{\sqrt{\frac{r}{R}}}_{\substack{\text{fraction of} \\ \text{trap. particles}}} k_\perp^2 \rho_b^2 \frac{e\Phi}{T_i}$$

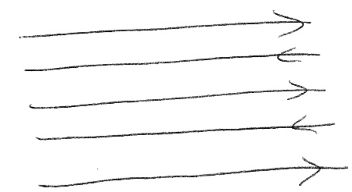
Hinton-Rosenbluth residual flow:

$$\frac{\Phi_{final}}{\Phi_{initial}} = \frac{k_r^2 \rho_i^2}{\sqrt{r/R}\, k_r^2 \rho_b^2 + k_r^2 \rho_i^2} = \frac{1}{1 + \frac{q^2}{\sqrt{r/R}} \frac{1}{f_{shaping}}}$$

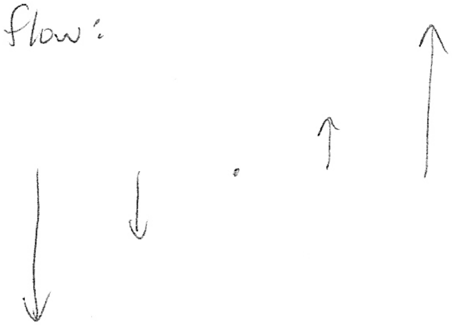
Implementation of Equilibrium-Scale ExB shear in GS2

Hammett, Dorland, Loureiro

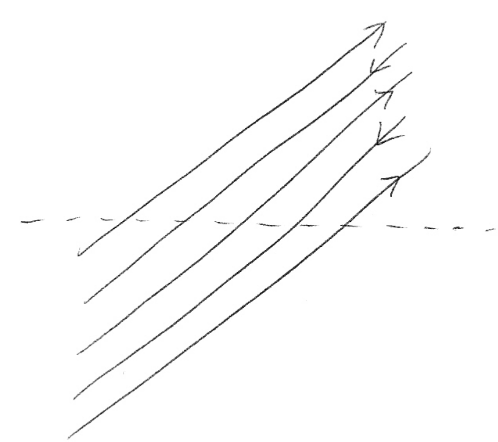
Eddies initially with $k_x = 0$:



+ sheared flow:



At a later time:



Now has finite

$$k_x = k_{x0} - k_y \frac{\partial v_y}{\partial x} t$$

GS2 solves Eq. of form:

$$\frac{\partial}{\partial t} f\left(k_x, k_y, \theta, E, \mu, t\right) = L\left(k_x, k_y, \theta, E, \mu\right) f\left(k_x, k_y, \ldots, t\right) + NonlinTerms$$

Include equilbrium scale ExB shear by substitution:

$$k_x \rightarrow k_x\left(t\right) = k_{x0} - k_y \frac{\partial \upsilon_y}{\partial x} t$$

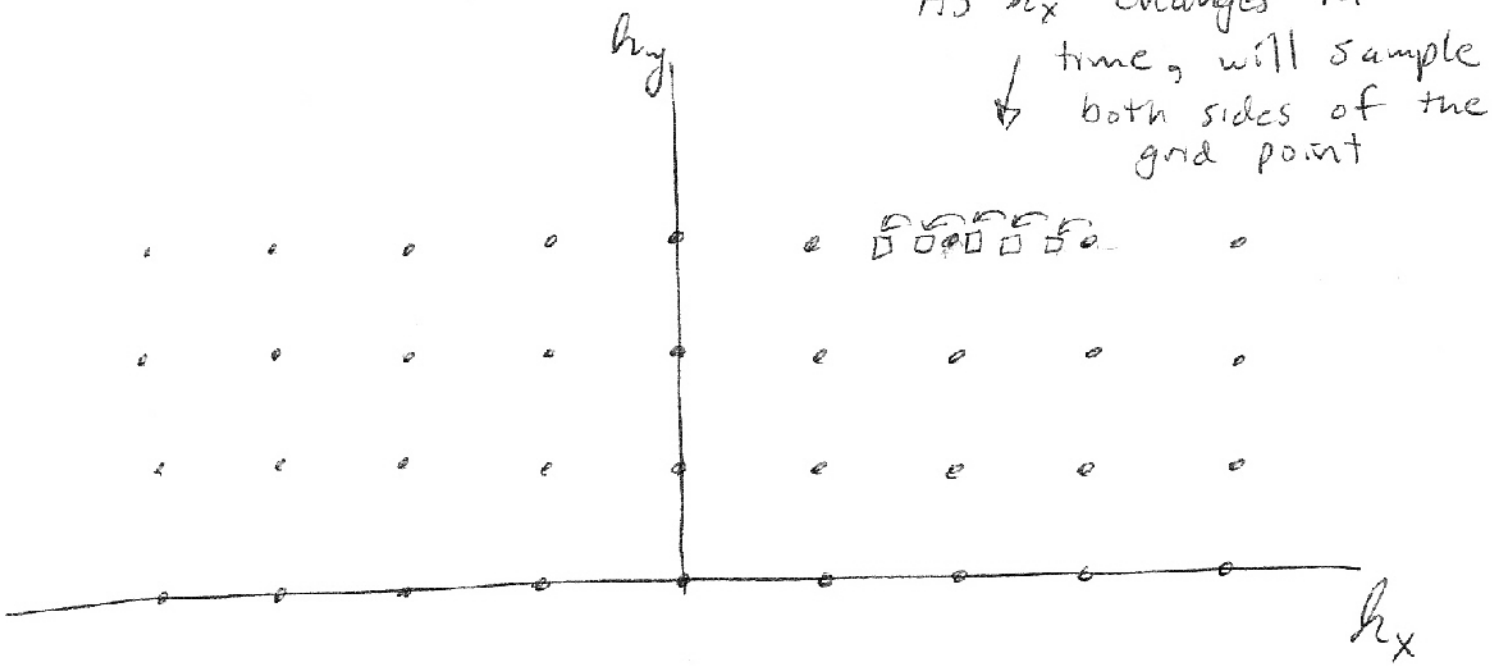
$$\frac{\partial}{\partial t} f\left(k_x(t), k_y, \theta, \ldots, t\right) = \underbrace{L\left(k_x(t), k_y, \theta, \ldots\right)} f\left(k_x(t), k_y, \ldots, t\right) + NonlinTerms$$

GS2 treats all linear terms implicitly. Recalculating all of the implicit response matrices every time step when k_x changes a little bit would be very expensive.

Instead of recalculating response matrices, just use Nearest-Grid-Point interpolations. Most easily implemented in reverse:

Whenever $k_x(t)$ differes from k_{x0} by more than $\Delta k_x/2$, shift f :

$$f\left(k_{xi}, k_y\right) \Leftarrow f\left(k_{xi} + \Delta k_x, k_y\right)$$



Errors will tend to cancel over time, making the method quasi-2cd order accurate.

(Like Nearest Grid Point NGP that is widely used in Gyrokinetic PIC codes, or somewhat like Godunov splitting).

(Could generalize to true 2cd order accuracy by doing 2 iterations per time step and interpolating.)

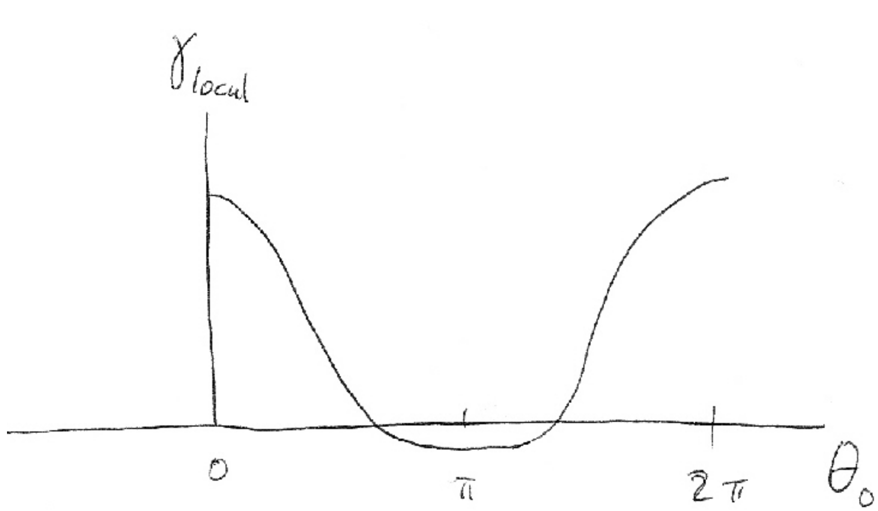
With sheared magnetic field:

$$k_x(t) = k_{xi} + k_y \hat{s}\,\theta - k_y \frac{\partial v_y}{\partial x} t$$

$$k_{xi} \equiv -k_y \hat{s}\,\theta_0$$

$$k_x(t) = k_y \hat{s}\,(\theta - \theta_0) - \underbrace{k_y \frac{\partial v_y}{\partial x} t}_{\text{E×B shear twists the eddy.}}$$

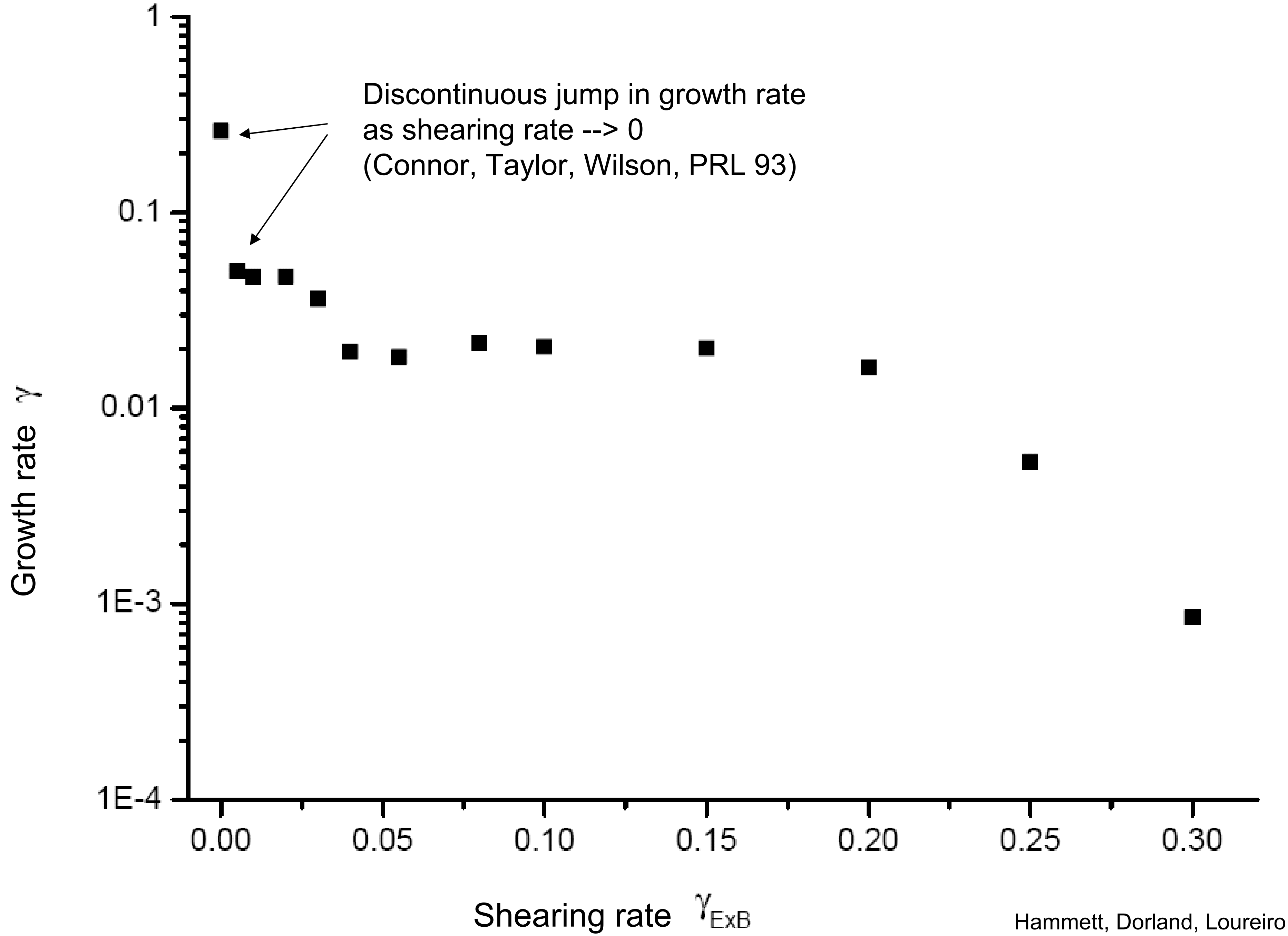
Can undo this twist by moving in θ along the sheared ~~mag~~ magnetic field.

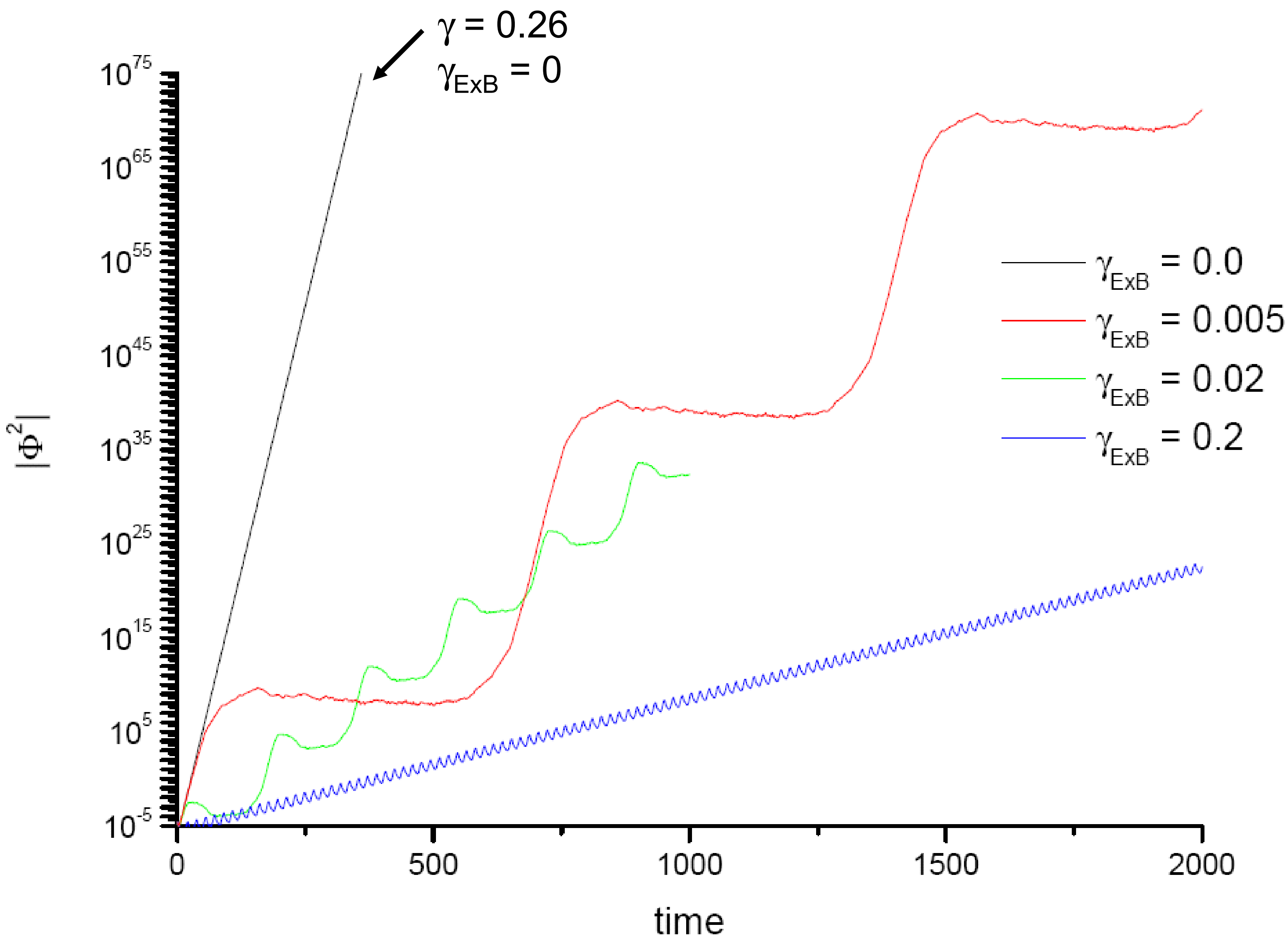


As mode moves along θ_0, the time-averaged growth rate changes discontinuously between

$$\gamma_{E\times B} = \frac{\partial v_y}{\partial x} = 0 \qquad V_{E\times B} \neq 0$$

But not really relevant if mode grows to nonlinear amplitude before moving out of the bad curvature region.


Discontinuous jump in growth rate
as shearing rate --> 0
(Connor, Taylor, Wilson, PRL 93)
1
0.1
0.01
1E-3
1E-4
Growth rate γ
0.00
0.05
0.10
0.15
0.20
0.25
0.30
Shearing rate γ_{ExB}
Hammett, Dorland, Loureiro



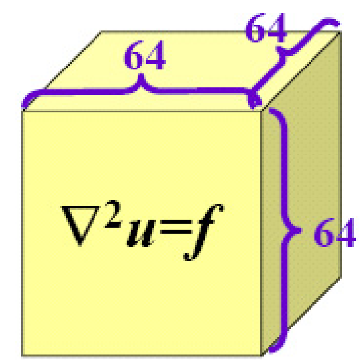
Floquet mode representation (Waltz, Dewar, Garbet 98) shows large growth of wave packet while in bad curvature region, even though time-averaged growth rate is small.

Hammett, Dorland, Loureiro

The power of optimal algorithms

- Advances in algorithmic efficiency can rival advances in hardware architecture
- Consider Poisson's equation on a cube of size $N=n^3$

Year	*Method*	*Reference*	*Storage*	*Flops*
1947	GE (banded)	Von Neumann & Goldstine	n^5	n^7
1950	Optimal SOR	Young	n^3	$n^4 \log n$
1971	CG w/ modified ILU	Reid / Gustafson (BIT 78)	n^3	$n^{3.5} \log n$
1984	Full MG	Brandt Multigrid	n^3	n^3



If n=64, implies
X16 Million speedup:
6 months -> 1 second

Restarted GMRES n^5

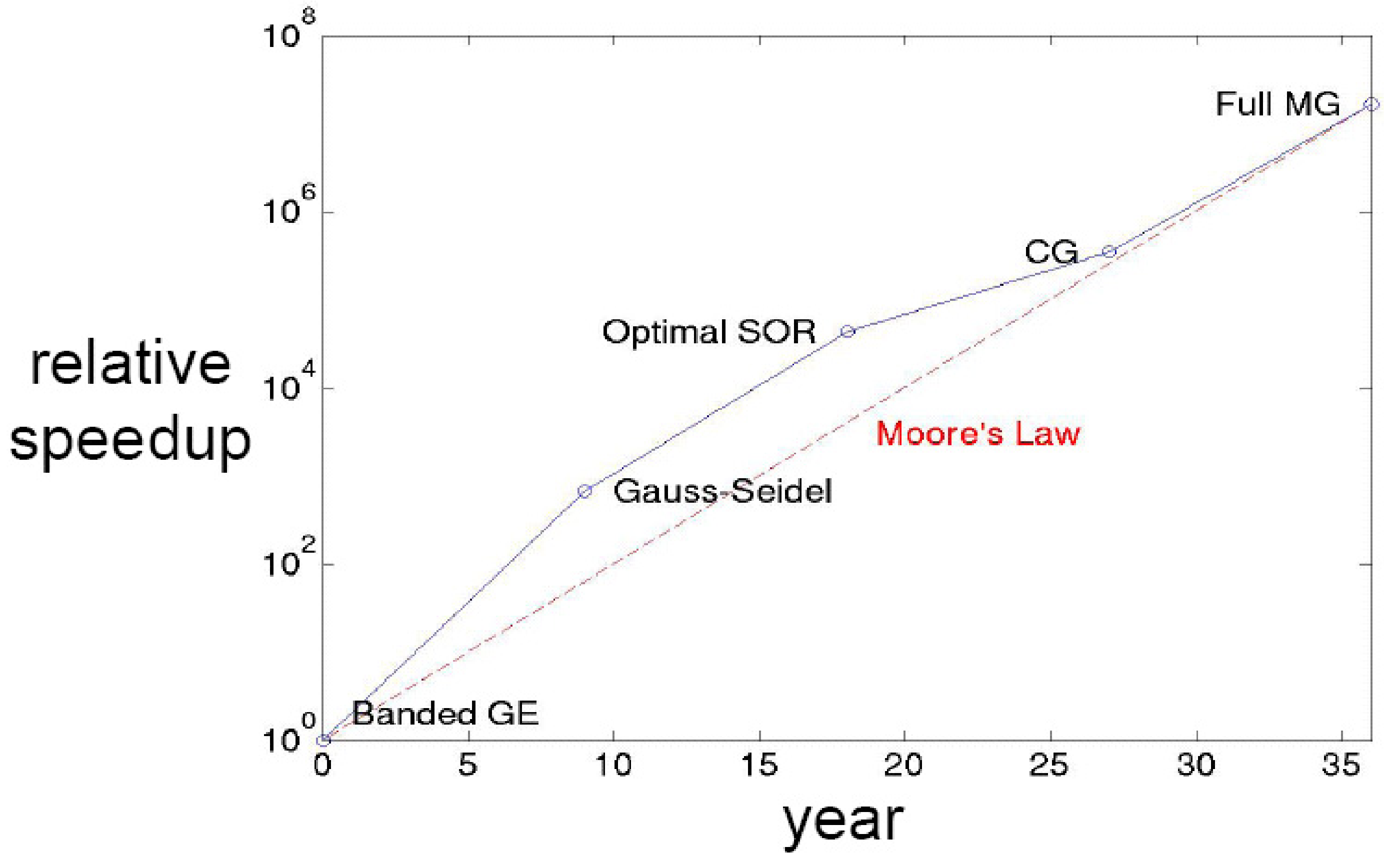
Loose GMRES/CG (Baker 2005) $\sim n^4$

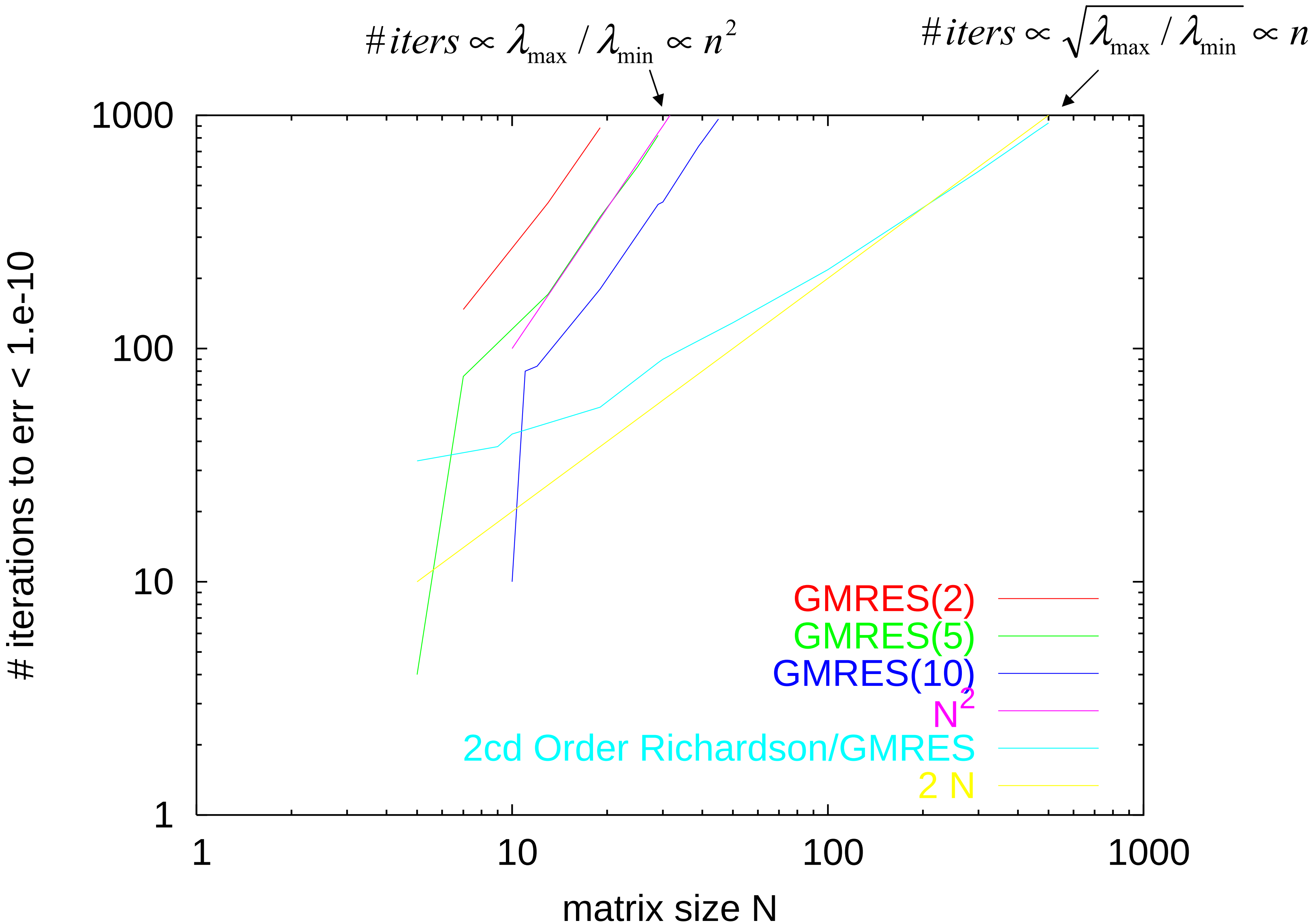
Loose GMRES/CG with modified ILU preconditioning $\sim n^{3.5}$

Based on David Keyes, Columbia Univ.

Algorithms and Moore's Law

- This advance took place over a span of about 36 years, or 24 doubling times for Moore's Law
- $2^{24} \approx 16$ million $\Rightarrow$ the same as the factor from algorithms alone!





1-D Poisson Problem: $\partial^2 \Phi / \partial x^2 = \rho$, with n grid points

Improved method for restarting GMRES

- "The Tortoise and the Hare Restart GMRES," Mark Embree (2003)
  http://epubs.siam.org/sam-bin/dbq/article/39961
  shows examples where GMRES(1) converges, GMRES(2) stagnates

- I developed a way to significantly improve restarted GMRES, by keeping information from previous search directions. Like "Dynamic Relaxation" (see Jardin's course notes), but time step & damping rate chosen optimally each iteration to minimize error. ("Dynamic Relaxation" = 2cd order Richardson iteration, related to 2cd order Chebyshev iteration). Nonlinear/Newton-Krylov.

  /u/hammett/codes/gmres/dr_gmres

- Turns out to be equivalent to LGMRES(1,1) "Loose GMRES":
  "A Technique for Accelerating the Convergence of Restarted GMRES", A. H. Baker, E. R. Jessup, T. Manteuffel, SIAM Journal on Matrix Analysis and Applications Volume 26, Number 4, pp. 962-984 (2005)

- Standard ILU preconditioning is of no benefit. Essential to use "Modified ILU" preconditioning, Gustafsson BIT 18, 142 (1978) (but MILU broken in Matlab)