Coarse Grained Roadmap for M3D Development

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Outline

- What kind of calculation can we do now in Extended MHD?
- How do the computational requirements scale to the kind of calculation we want (need) to do?
- How do we get there from here?

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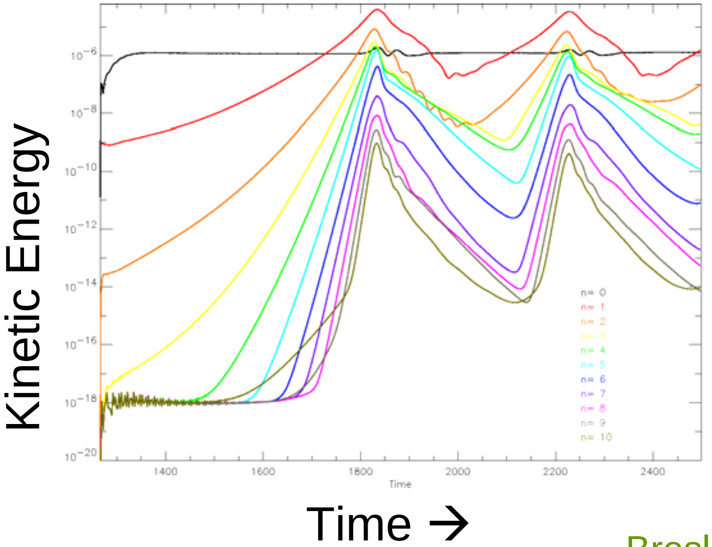
What Kind of Calculation can we do now in Extended MHD?

- M3D and NIMROD have been involved in a nonlinear benchmark on CDX-U
- The most recent M3D simulation used:
  - 10,000 x 50 = 500,000 elements
  - 400,000 time steps
  - ~2 x 10^{11} space time points

  (probably under-resolved)



Breslau

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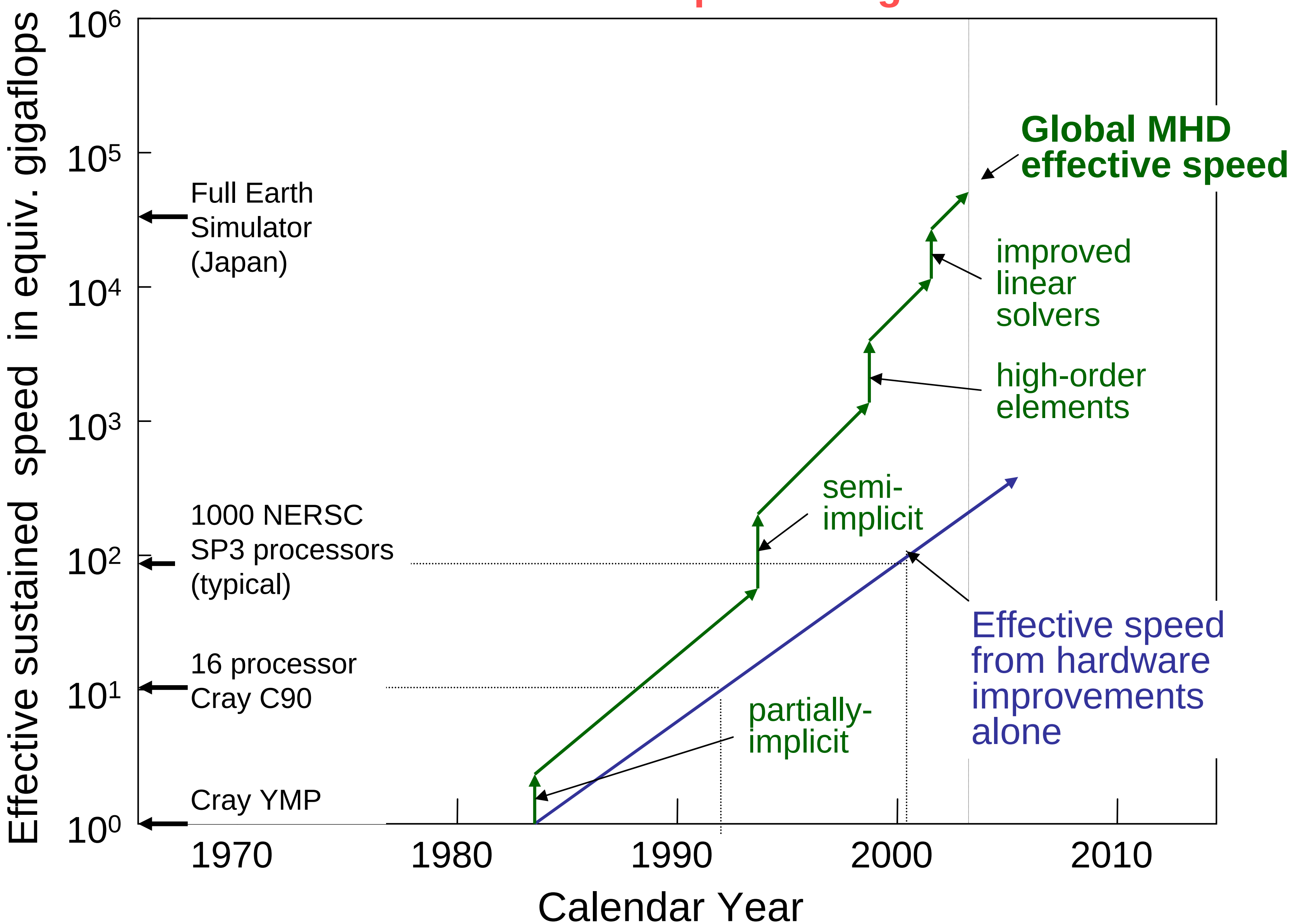
Straightforward Extrapolation from CDX-U to ITER

name	symbol	units	CDX-U	DIII-D	ITER
Field	B_0	Tesla	0.22	1	5.3
Minor radius	a	meters	.22	.67	2
Temp.	T_e	keV	0.1	2.0	8.
Lundquist no.	S		1×10^4	7×10^6	5×10^8
Mode growth time	$\tau_A S^{1/2}$	s	2×10^{-4}	9×10^{-3}	7×10^{-2}
Layer thickness	$aS^{-1/2}$	m	2×10^{-3}	2×10^{-4}	8×10^{-5}
zones	$N_R\times N_\theta\times N_\phi$		3×10^6	5×10^{10}	3×10^{13}
CFL timestep	$\Delta X/V_A$ (Explicit)	s	2×10^{-9}	8×10^{-11}	7×10^{-12}
Space-time pts			6×10^{12}	1×10^{20}	6×10^{24}

In the past, “Effective speed” increases came from both faster hardware and improved algorithms



How to get an additional 12 orders of magnitude in 10-15 years?

- 1.5 orders: increased parallelism
- 1.5 orders: processor speed and efficiency
- 4 orders: adaptive gridding
- 1 order: higher order elements
- 1 order: field-line following coordinates
- 3 orders: implicit algorithms

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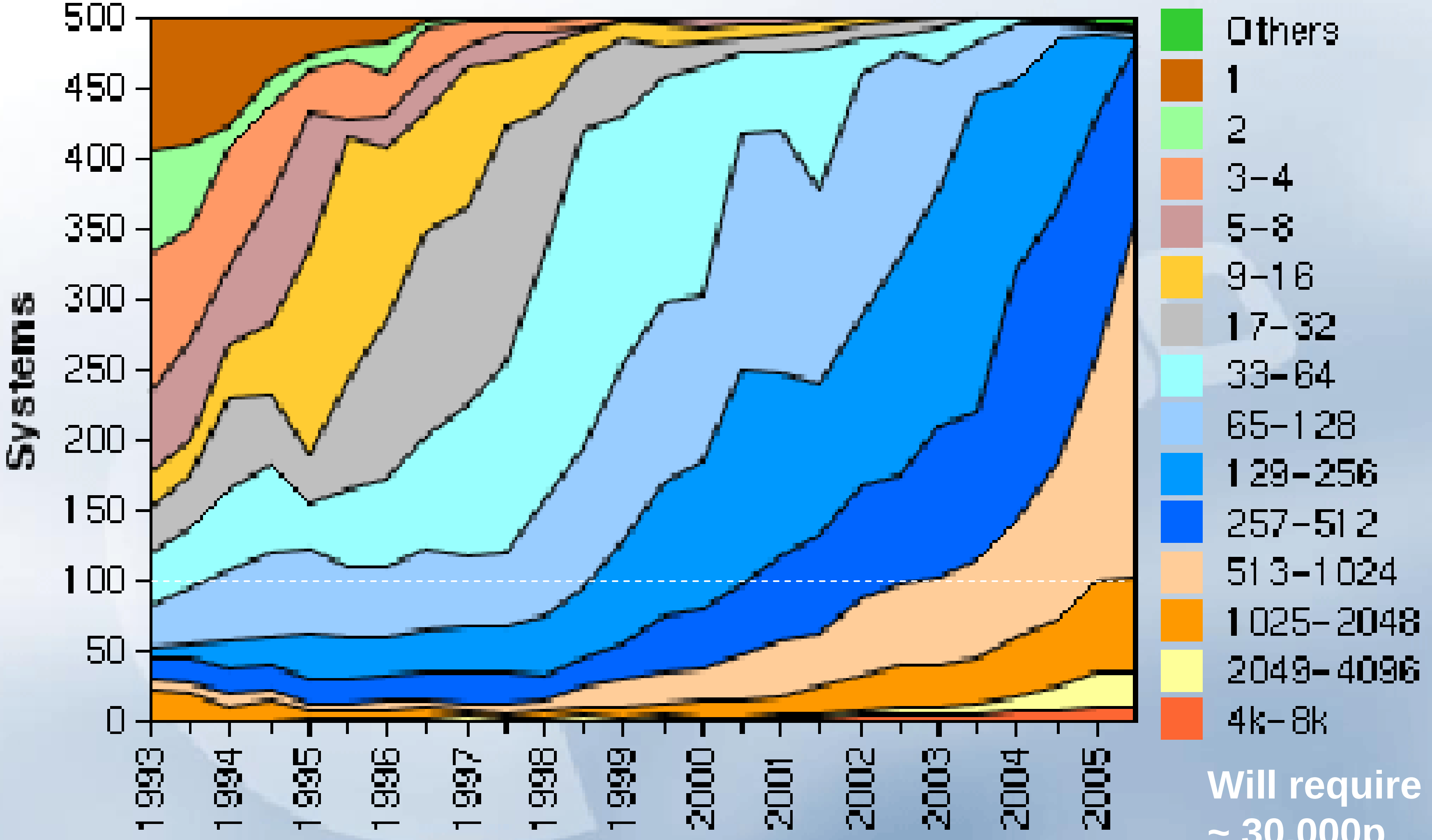
1.5 orders: increased parallelism

of processors in the top 500 computers vs year:

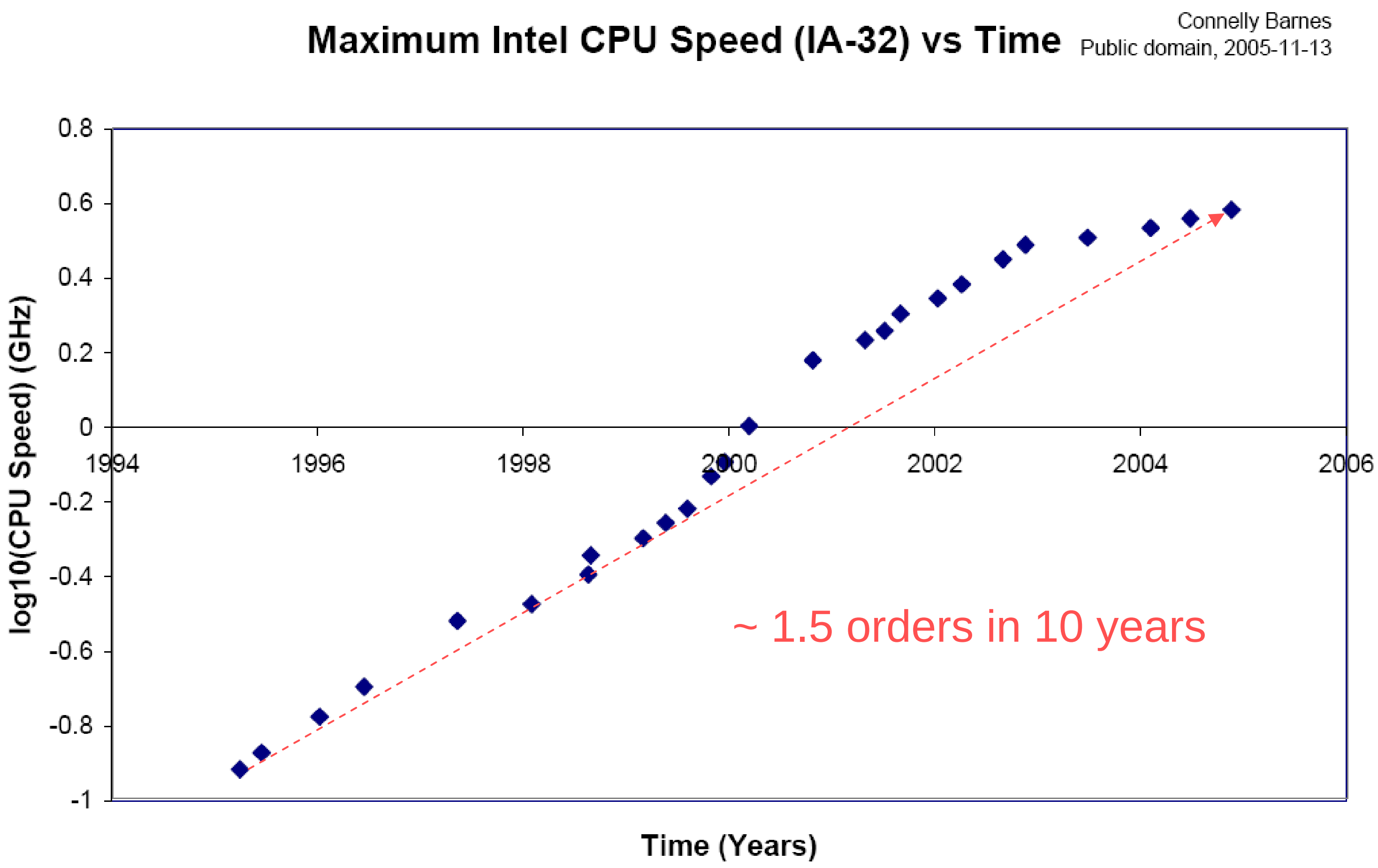


Will require ~ 30,000p

100th fastest went from 30p to 1000p in 12 years

http://www.top500.org/

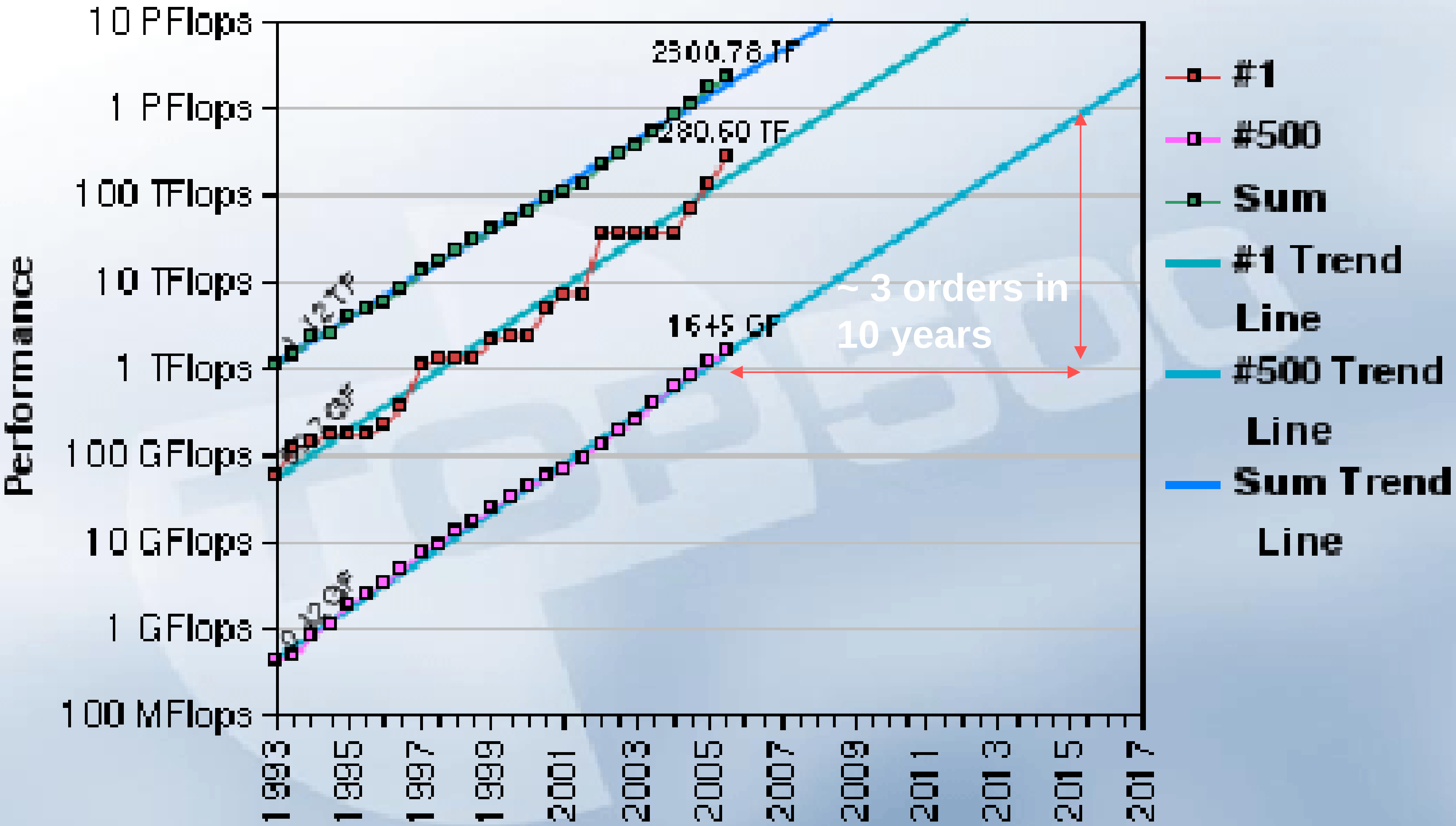
1.5 order: processor speed and efficiency



Also, improved compilers, chip-design, memory busses, etc. will lead to greater usable percent of peak performance (now ~5%)

TOP500 SUPERCOMPUTER SITES

Projected Performance Development



Combined processor speed + parallelism

4 orders: adaptive gridding

$(V, \Delta R) =$ volume and typical mesh spacing in bulk of plasma

$(v, \Delta r) =$ volume and mesh spacing in refinement region (assuming 1D boundary layer):

Number of zones required: $N = \dfrac{V - v}{(\Delta R)^3} + \dfrac{v}{(\Delta R)^2(\Delta r)} \sim \dfrac{1}{(\Delta R)^2}\left[\dfrac{V}{(\Delta R)} + \dfrac{v}{(\Delta r)}\right]$

Ratio of improvement: $\dfrac{\mathrm{V}/(\Delta r)^3}{\dfrac{1}{(\Delta R)^2}\left[\dfrac{V}{(\Delta R)} + \dfrac{v}{(\Delta r)}\right]} = \dfrac{1}{\left(\dfrac{\Delta r}{\Delta R}\right)^2\left[\left(\dfrac{\Delta r}{\Delta R}\right) + \dfrac{v}{V}\right]}$

For ITER, we can estimate : $\dfrac{v}{V} \sim \dfrac{\Delta r}{\Delta R} = 10^{-2}$

This gives $= N \sim \dfrac{1}{\left(\dfrac{\Delta r}{\Delta R}\right)^2\left[\left(\dfrac{\Delta r}{\Delta R}\right) + \dfrac{v}{V}\right]} \sim 5\times 10^5$

Thus, 4 orders may be conservative!

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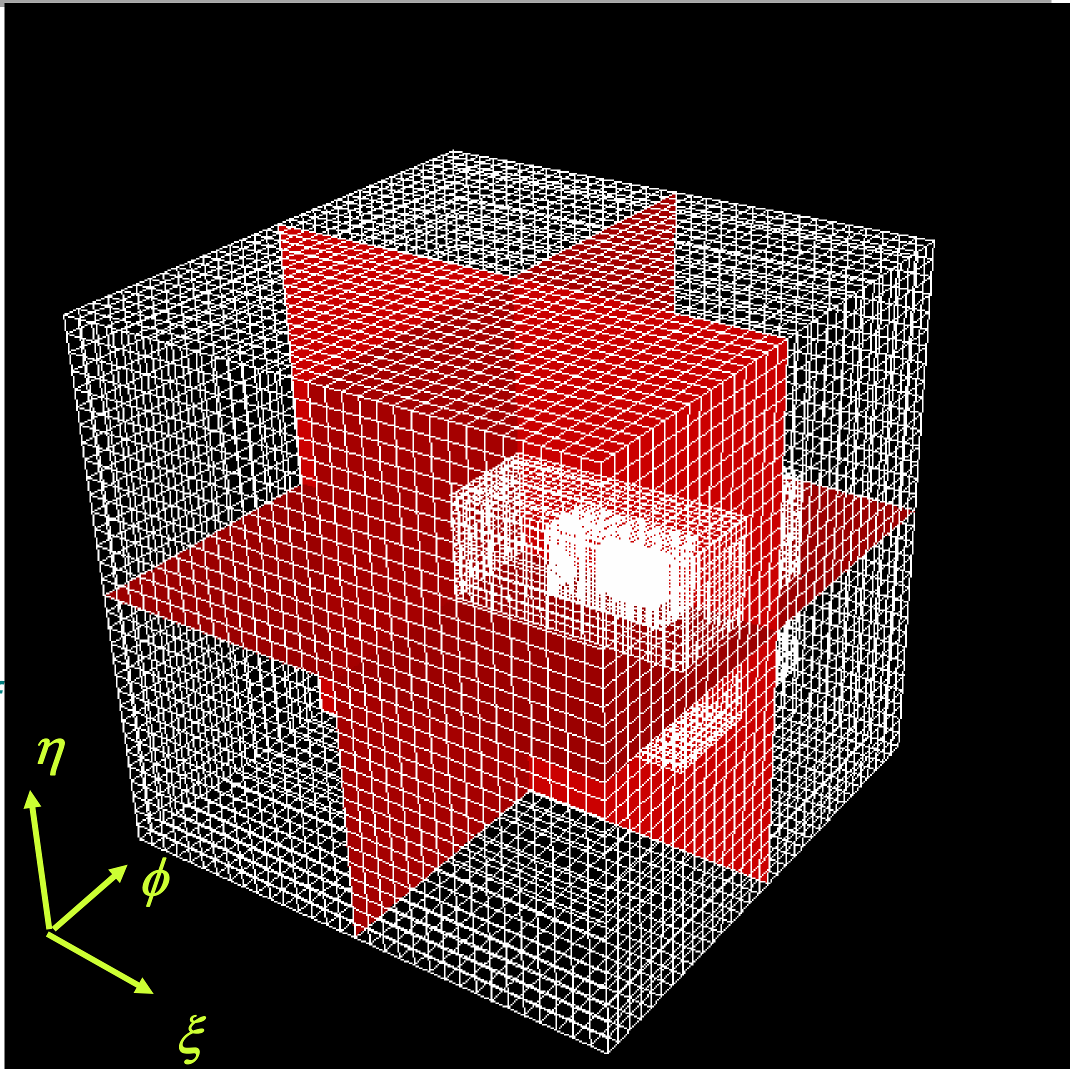
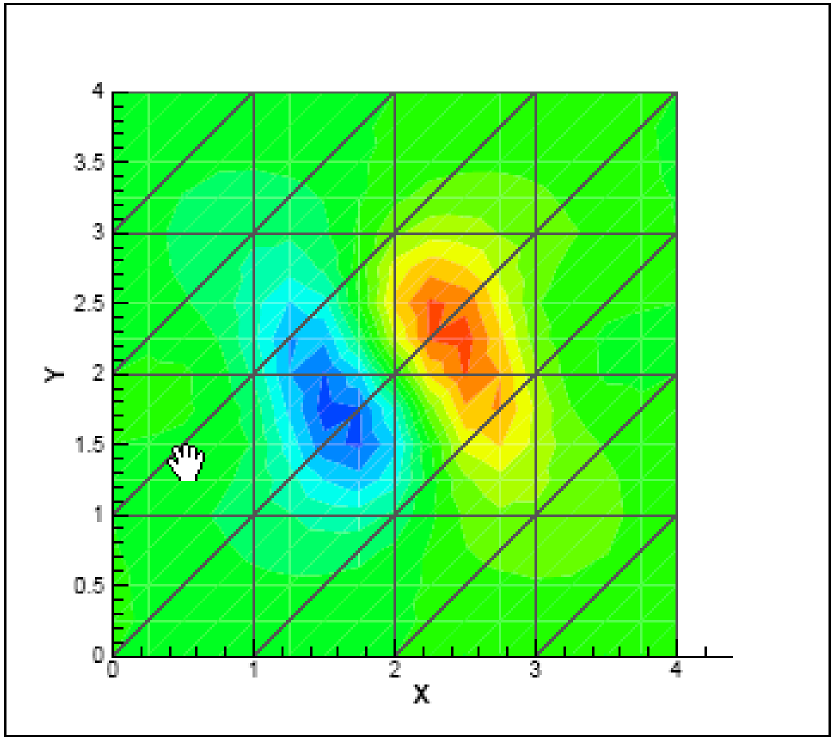
Eg: Use of AMR in pellet injection simulations

- Meshes clustered around pellet
- Computational space mesh structure shown on right
- Mesh stats
  - *32^3 – base mesh with 5 levels, and refinement factor 2*
  - *Effective resolution: 1024^3*
  - *Total number of finite volume cells:113408*
  - *Finest mesh covers 0.015 % of the total volume*
  - *Time adaptivity:*
    $1\ (\Delta t)_{base} = 32\ (\Delta t)_{finest}$

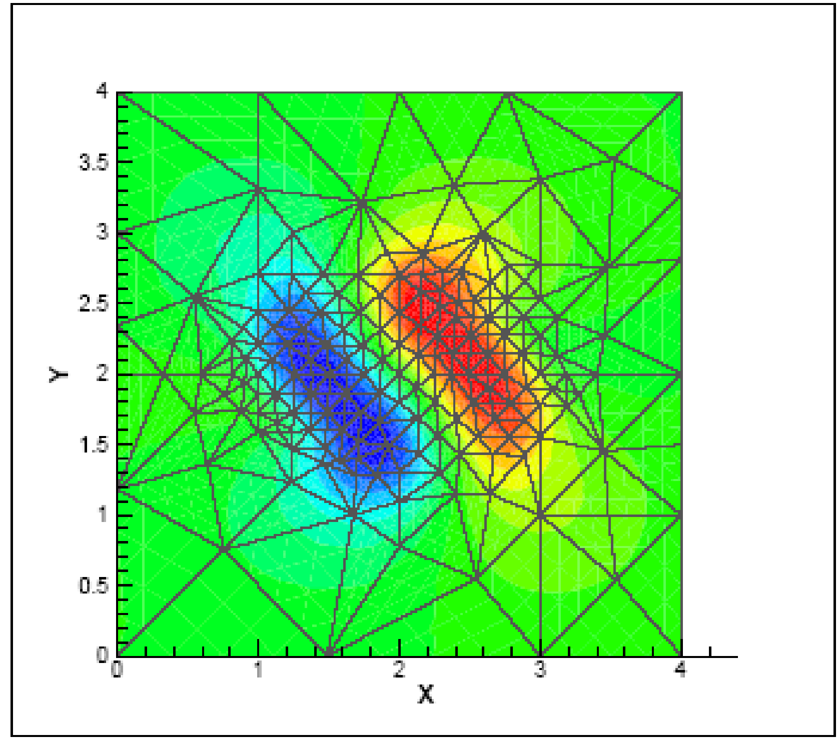
~ 4 orders already demonstrated in pellet injection simulations



Eg: Unstructured Adaptive Meshing being developed



(a) Initial mesh



(b) Adapted mesh

Bauer

Andy Bauer (RPI) has implemented an arbitrary Adapted Mesh in the M3D-C^1 code and is exploring different adaptive strategies

1 order: High order elements

- Same accuracy can be obtained with many fewer elements and less work
- Eg: in 2D, compare work required for linear elements and reduced quintic elements for same accuracy to solve : $\nabla^4 \Phi = 0$ in 2D

Number of elements	Matrix rank	Ratio of elements	ratio N=10	ratio N=100	ratio N=1000
N	$4N^2$	$(1/9)N^{6/5}$	1.7	30	440
$N^{2/5}$	$36N^{4/5}$	1			

Thus, 1 order may be conservative!

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1 order: field-line following coordinates

- Mode structure largely follows field lines, and much less resolution is required along than across field: $\vec{B} \bullet \nabla \sim 0$

- Making the toroidal coordinate an (approximate) field-line-following coordinate can greatly relieve resolution requirements in that direction

- GTC code found a savings of 100 through this technique!

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3 orders: implicit algorithms

- For ITER, the mode growth time is nine orders longer than the CFL timestep based on the Alfven wave:

$$\gamma^{-1} \sim 7\times10^{-2} \text{ vs } \Delta t_{\mathrm{CFL}} \sim 7\times10^{-12}$$

- For accuracy, you need the mode growth resolved into a number of timesteps that is determined by the temporal order of the implicit temporal discretization.

$$T_{\Delta} \sim (\Delta t)^2 \gamma^2 \quad \Rightarrow \Delta t_{implicit} = .01\gamma^{-1} \sim 10^{-3} \text{ should be adaquate}$$

- Assume that you lose about two-three orders of magnitude due to the cost of solving nonlinearly implicit problems on each time step. (assumes about 3 Newton steps with 30-60 Krylov steps on each one.

- Net win is: $\dfrac{1}{1000} \times \dfrac{\Delta t_{implicit}}{\Delta t_{CFL}} =\sim 10^5$

Again, estimate of 3 orders may be conservative

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Summary: How to get an additional 12 orders of magnitude in 10-15 years?

- 1.5 orders: increased parallelism
- 1.5 orders: processor speed and efficiency
- 4 orders: adaptive gridding
- 1 order: higher order elements
- 1 order: field-line following coordinates
- 3 orders: implicit algorithms

Should be possible. Requires manpower to implement and customize mostly known algorithms in leading codes

Note: Hardware (3) : Software (9) !!

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Additional thoughts

- Such a large separation between time-scales and space-scales suggest that some multi-scale mathematics (or asymptotics) techniques might be applicable.
- We encourage people to explore developing new equations sets that are free of the large scale separation, yet asymptotically correct.