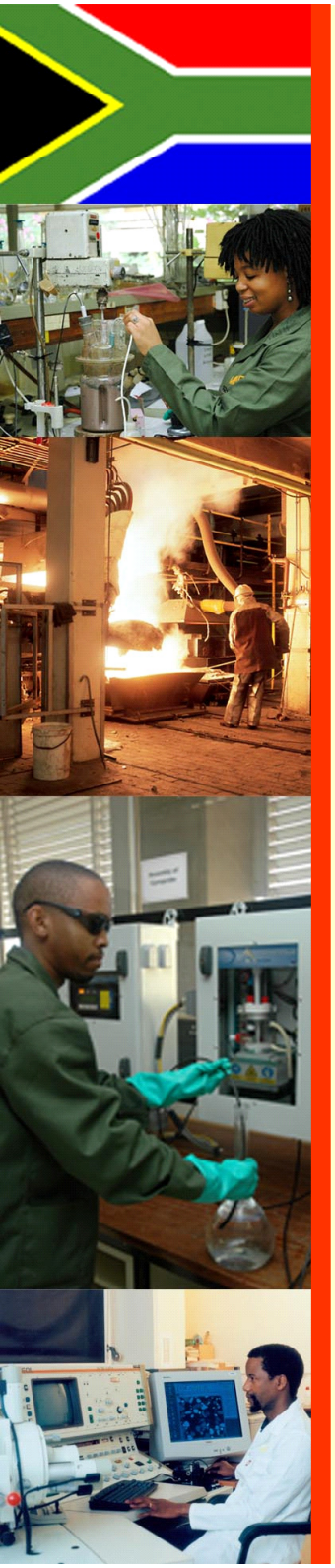

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Arc Modelling
or:
How I Learned To Stop Worrying And Love The Supercomputer

QG Reynolds

Pyrometallurgy Division, Mintek

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Introduction

- Pyrometallurgy process design presents many challenging problems for computational modelling
- Heat transfer, fluid dynamics, electromagnetics, phase change, multiphase flow, free surface flow, granular flow, thermo-chemistry…
- …often all at the same time!

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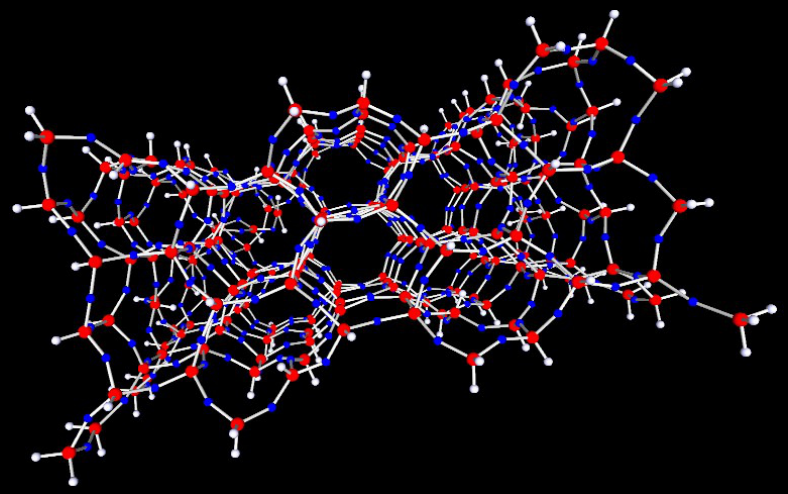
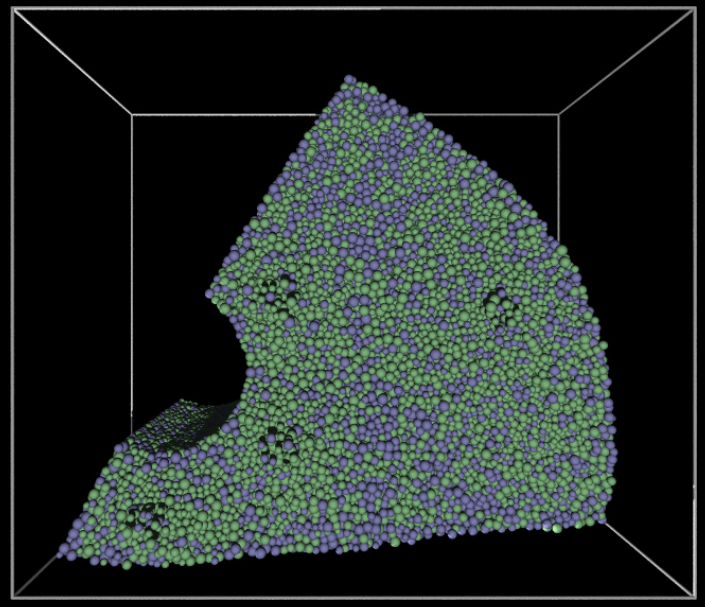
Using HPC for Pyrometallurgy

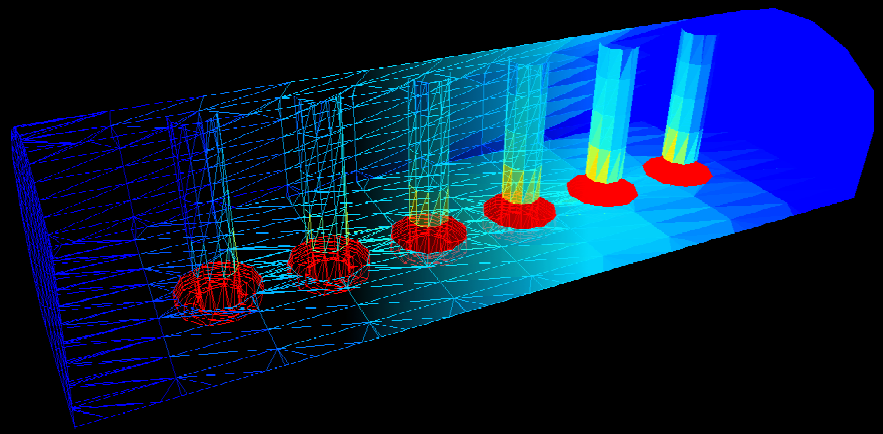
Molecular Modelling



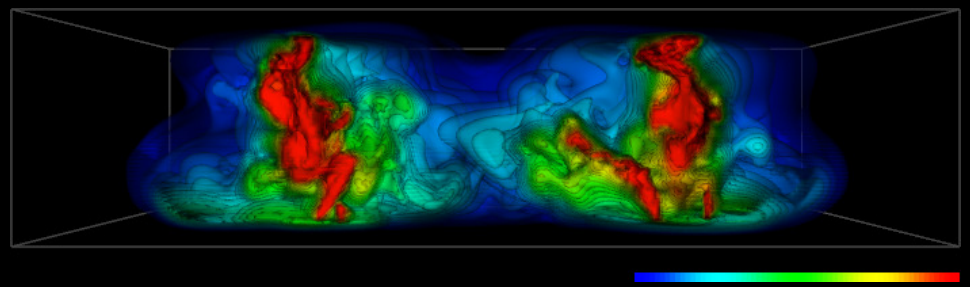
DEM - Granular Flows



Thermal Radiation



CFD/MHD - Arc Modelling



Arc Modelling – Why?

- Plasma arcs are a key heating and stirring element in DC arc furnaces and open-arc AC furnaces
- The arc environment is extremely harsh
  - Heat, electromagnetic radiation and interference, dust
  - Difficult to do measurements!
- High fluid velocities and large EM forces result in very rapid motion and evolution of the arc (<< 1 ms)

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Arc Modelling – Why?

Current: 3 kA

Arc length: 35 cm

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Arc Modelling – How?

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} + \nabla p = \nu \nabla^2 \mathbf{v} + \frac{\mathbf{j} \times \mathbf{B}}{\rho}$$

$$\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T = \alpha \nabla^2 T - \frac{Q_R}{\rho C_P} + \frac{\mathbf{j} \cdot \mathbf{j}}{\sigma \rho C_P}$$

$$\nabla \cdot (\sigma \nabla \phi) = 0$$

$$\mathbf{j} = -\sigma \nabla \phi$$

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{j}$$

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Arc Modelling – How?

- Temporal discretisation (velocity and temperature)
  - Explicit: 4th order Runge-Kutta + fractional time-step
  - Stability guaranteed under CFL condition
- Spatial discretisation (all fields)
  - 2D and 3D FD on cartesian mesh
  - Simple stencil, very easy to parallelise
  - Spectral-transform and Multigrid intermediate solvers
- Method permits scaling to very high spatial and temporal resolutions needed for fully resolved results (>10^8 DOF)

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Arc Modelling – What?

- Small scale (lab and pilot plants)
  - DC arcs, <1kA current, <10cm arc length
  - Gas space between electrode tip and bath surface
- Arc initiation and formation
- Variations in dynamics with process parameters
- Multiple arcs and their interactions
- Reverse-polarity arcs
- Brush arc conditions
- Composition of gas environment
- etc…

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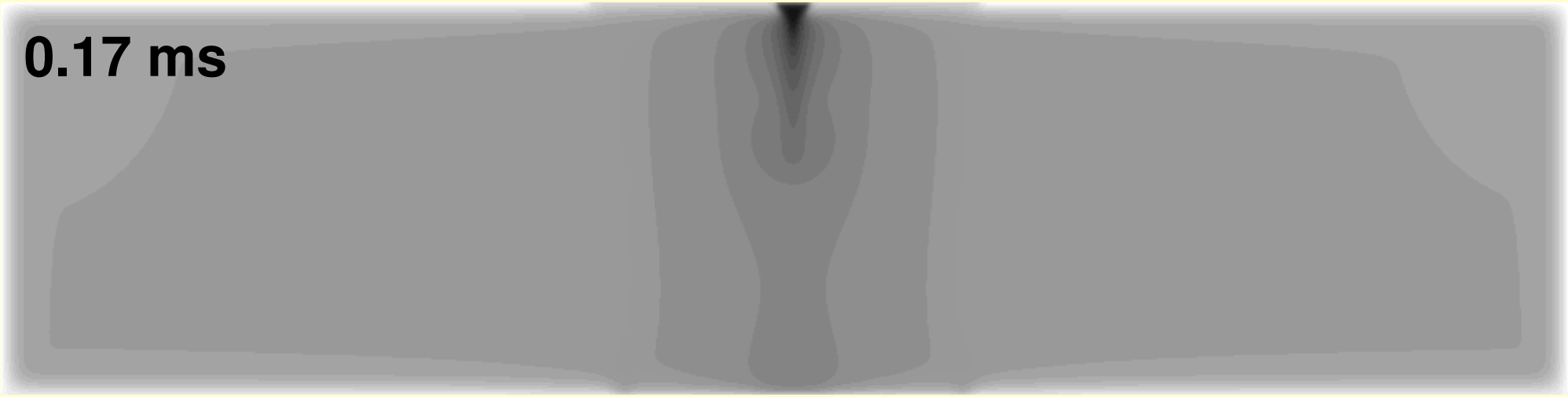
Arc Formation



- Arc in air: 500A, 5cm length, initial temperature 10000 K, initial velocities zero
- Temperature plot, scale 2000 (white) to 15000 K
- Hot arc jet forms, directed away from cathode spot on electrode surface at top

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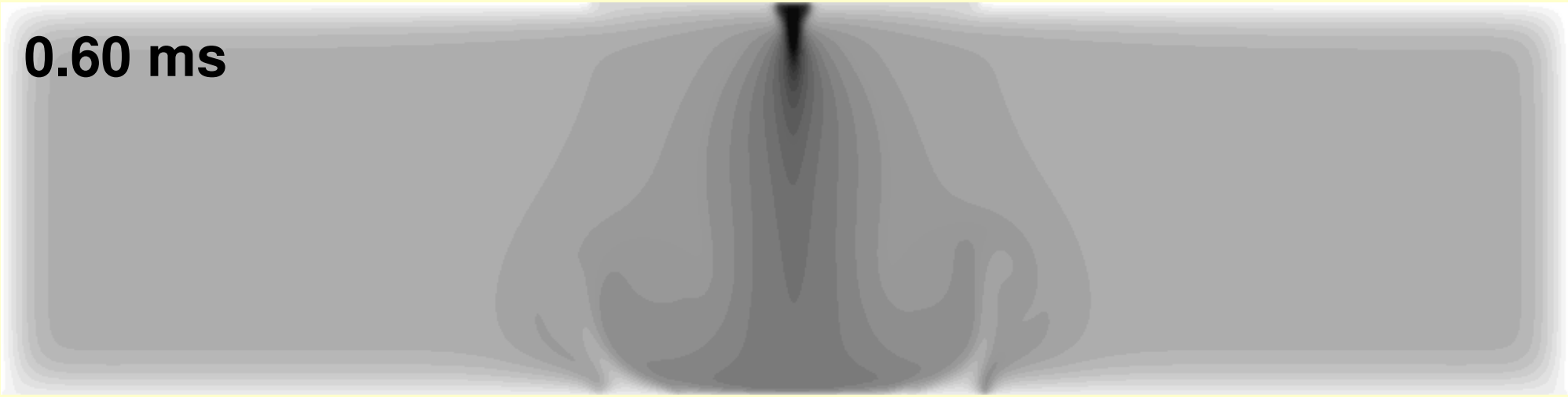
Arc Formation



- Temperature plot, scale 2000 (white) to 15000 K
- Initial arc column retains left-right symmetry for a short time into the simulation

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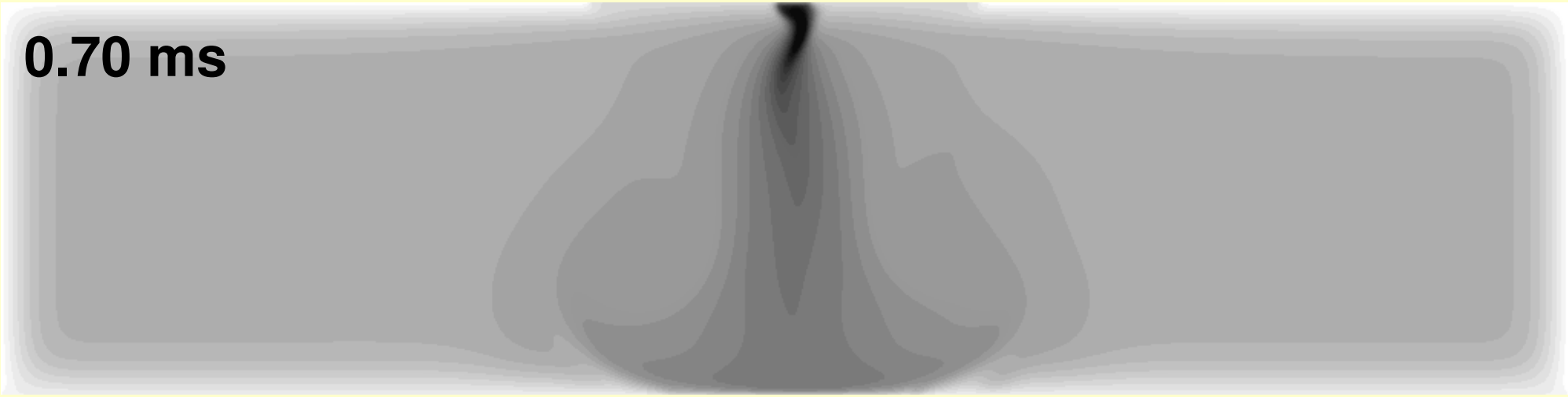
Arc Formation



- Temperature plot, scale 2000 (white) to 15000 K
- Symmetry breaks, with oscillations originating near the cathode spot

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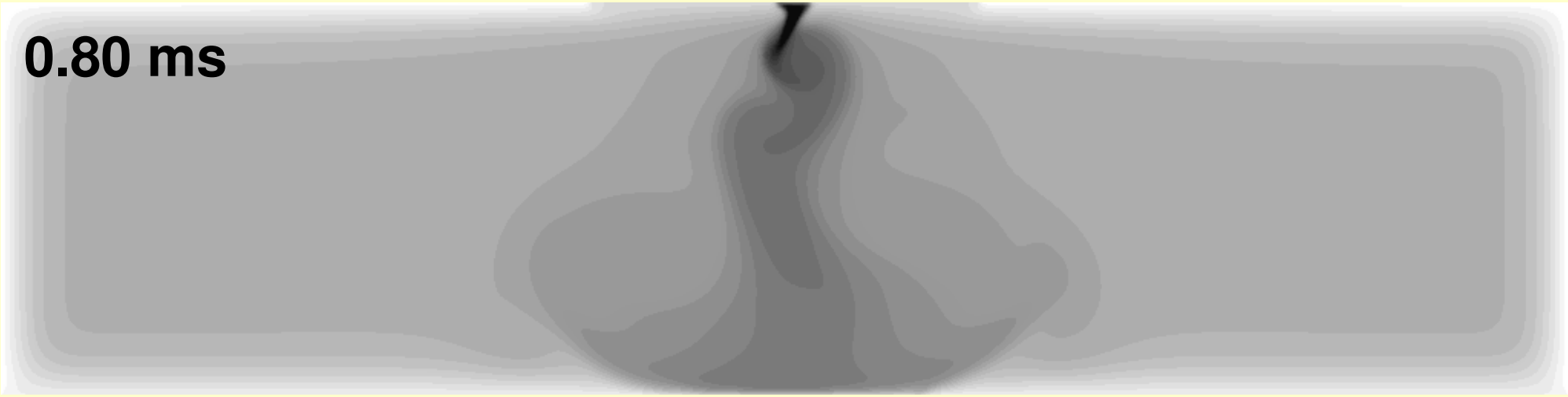
Arc Formation



- Temperature plot, scale 2000 (white) to 15000 K
- Oscillations drive further chaotic instability of the arc column

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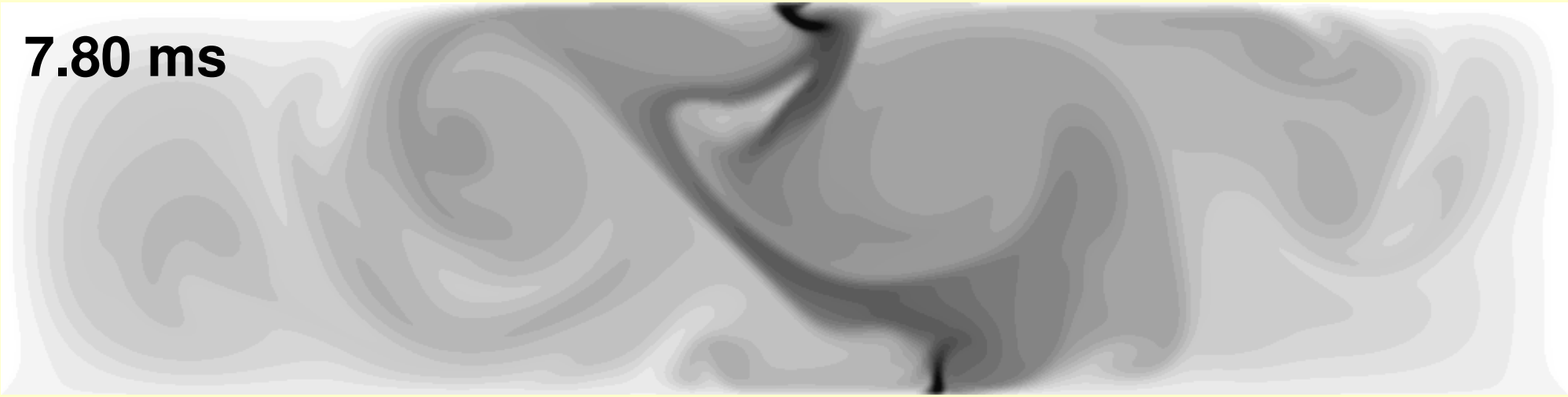
Arc Formation



- Temperature plot, scale 2000 (white) to 15000 K
- As the system evolves, the strong coupling between the fluid flow and EM fields causes complex shapes to develop in the arc column

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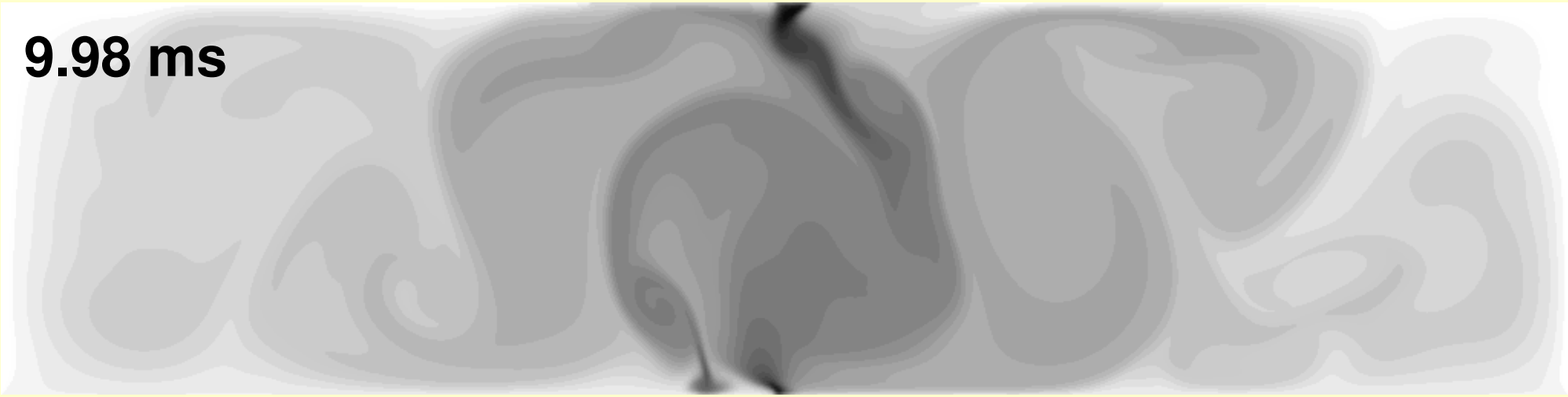
Arc Formation



- Temperature plot, scale 2000 (white) to 15000 K
- Spontaneous, short-lived arcs frequently form on the anode surface (at bottom)
- This phenomenon also seen in high speed imaging

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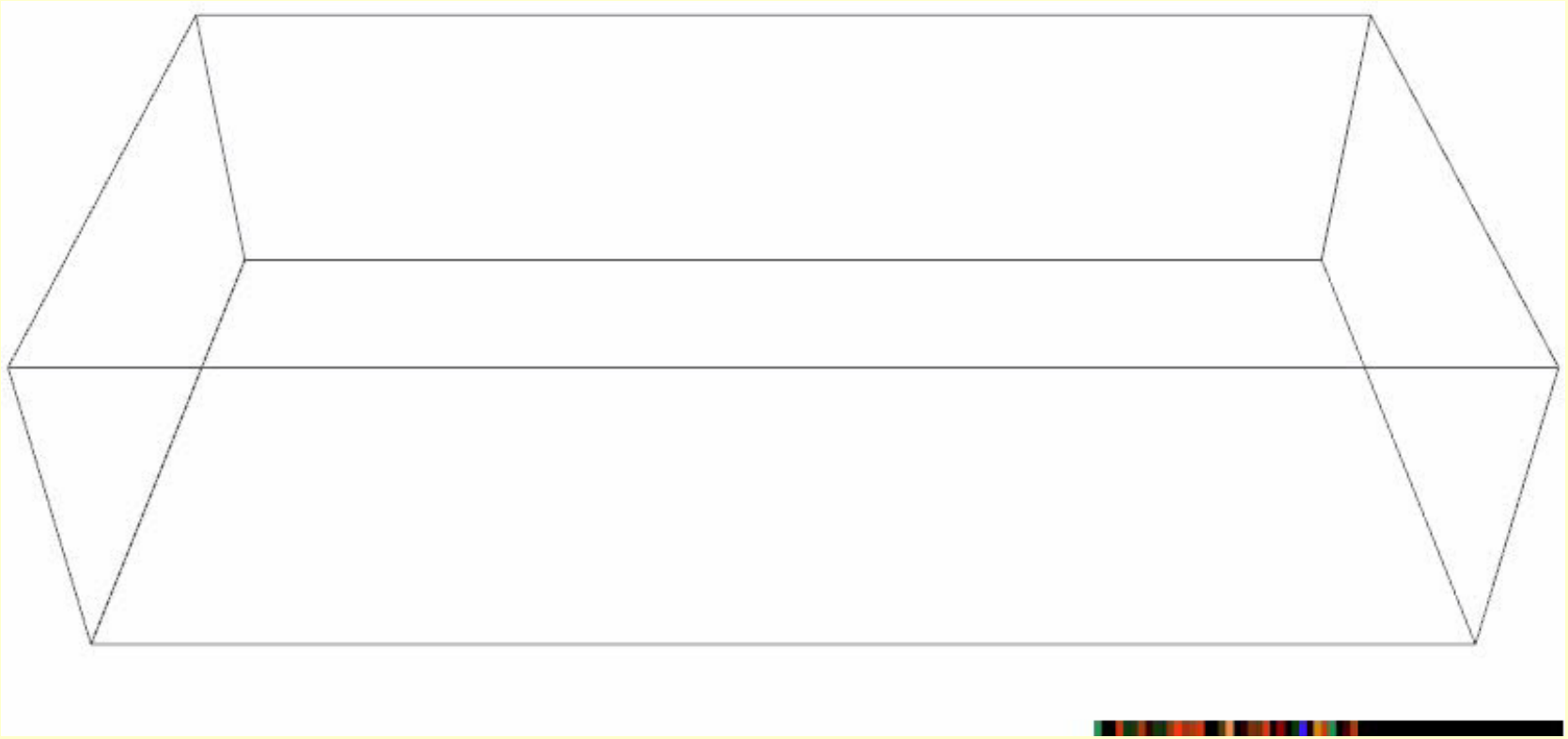
Effect of Current on Arc Behaviour



- Arcs in air: 100A (left), 250A (right), 5cm length, initial temperature 10000 K, initial velocities zero
- Velocity magnitude plot, scale 0 to 100 m/s
- Stable jet transitions to regular oscillations

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Effect of Current on Arc Behaviour

- Arcs in air: Both at 500A, 5cm length, initial temperature 10000 K, initial velocities zero
- Velocity magnitude plot, scale 0 to 100 m/s
- Chaotic instabilities

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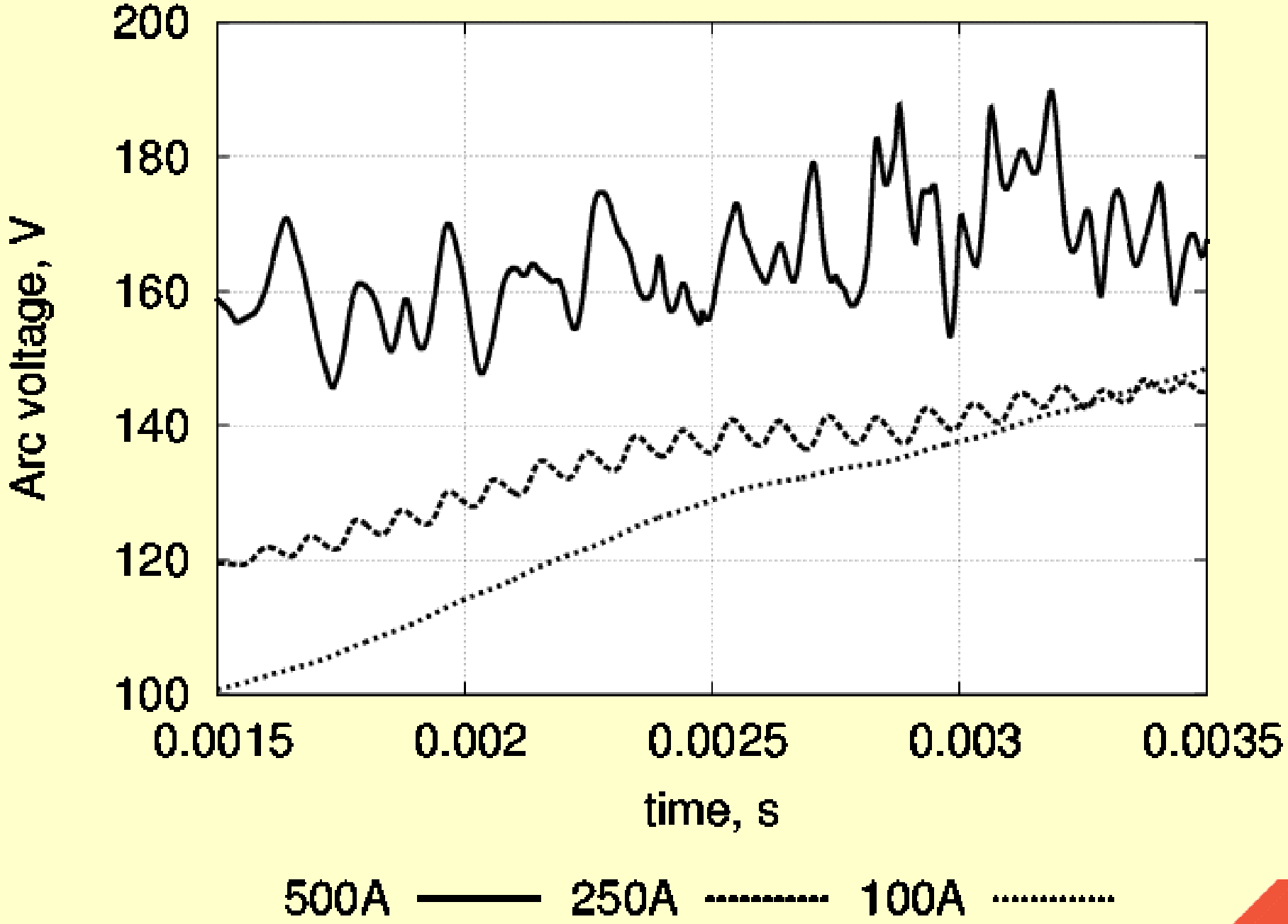
Effect of Current on Arc Behaviour



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Arc Modelling and HPC

- All well and good, we can successfully run fully resolved models of small arcs (~0.5kA, ~5cm)
- This still requires substantial computer power, around 40-50 GigaFLOPS
- What we'd *really* like to do is run the same models for industrial scale arcs (~50kA, ~50cm)
- …but why is that important, and what would we need to do it?

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Virtual Prototyping – A Case Study

- Automotive industry vehicle impact safety testing (1910s – 1981)

  - Build a physical prototype of proposed new product
  - Crash test it
  - Feed back crash test data into new prototype
  - Iterate until product safety quality is met

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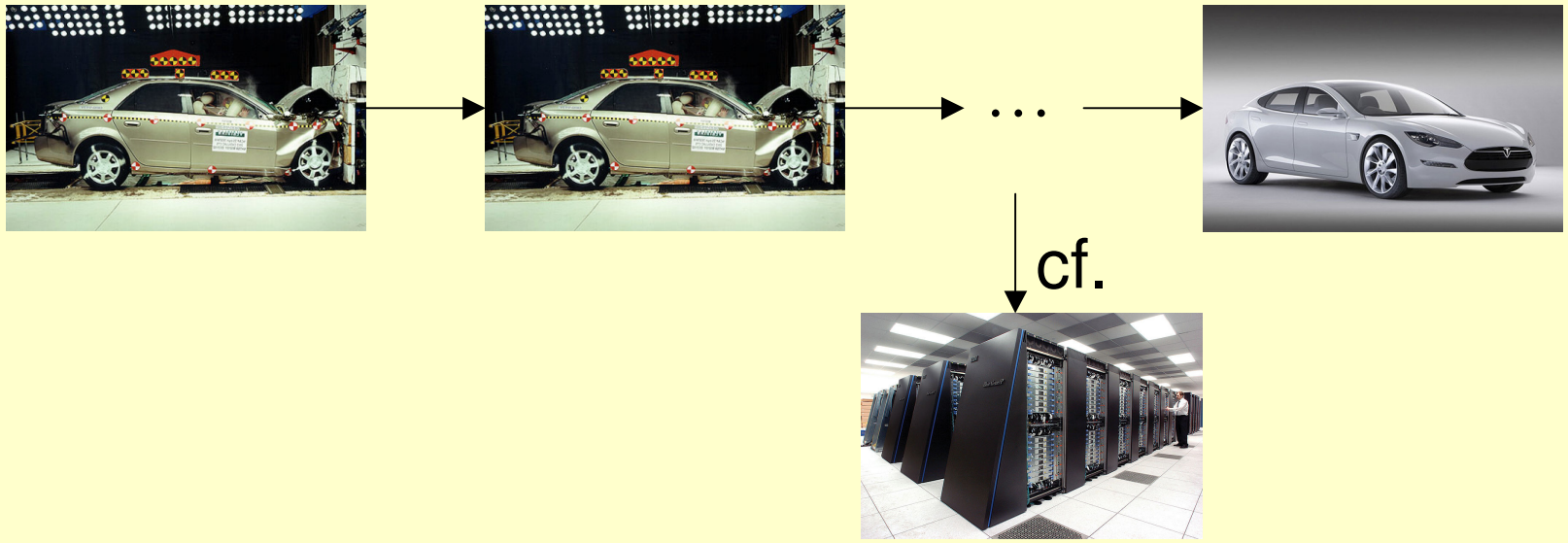
Virtual Prototyping – A Case Study

- Automotive industry vehicle impact safety testing (1981 – 1986)



  - Computational stress and deformation analysis becomes possible for individual, monolithic vehicle components
  - Product development pipeline unchanged, just complemented by comparison with models

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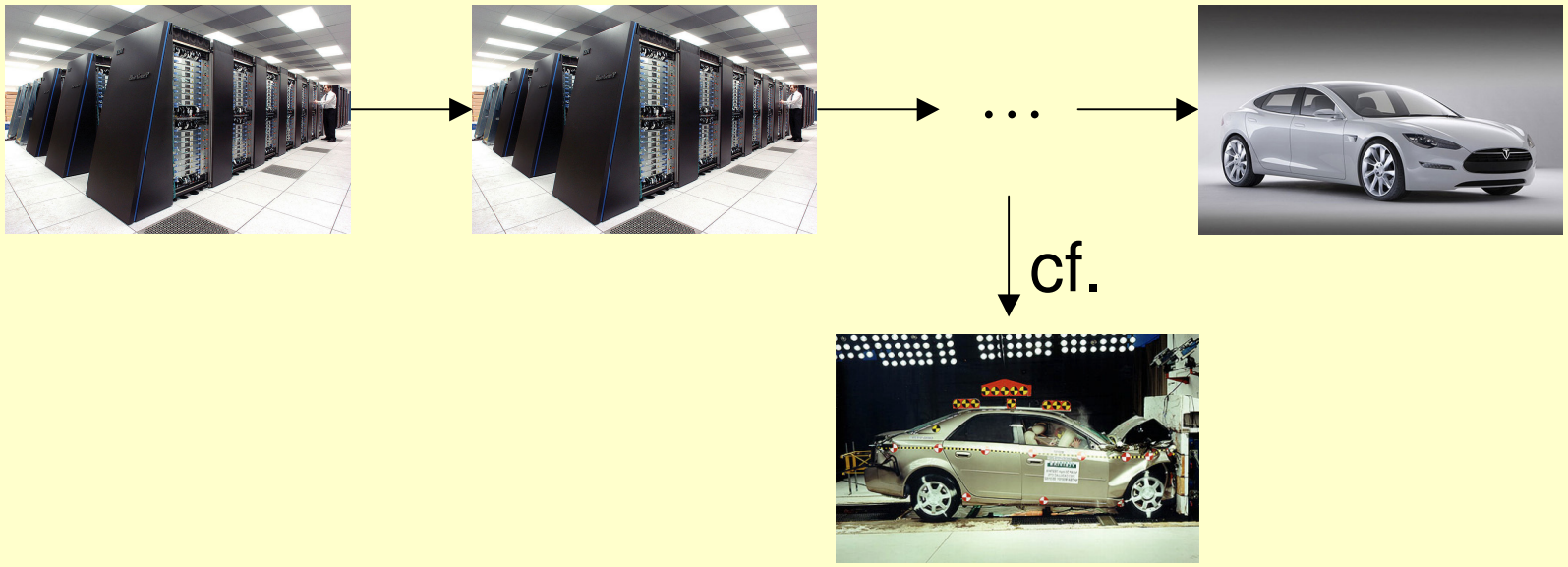
Virtual Prototyping – A Case Study

- Automotive industry vehicle impact safety testing (1986 – present)



  - Computational FEA can accurately simulate an entire multicomponent vehicle model
  - Development pipeline changes radically – “more tests, better quality, in less time, for less money”

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Arc Modelling and HPC

- Szekely et al and our present work both suggest arc velocities scale approximately proportional to I, so $v_{50kA} \approx 100\ v_{0.5kA}$
- Dimensions of region also increase, $X_{50cm} = 10\ X_{5cm}$
- Industrial scale therefore increases Re by 1000x
- In 3D, linear mesh density required for fully resolved flow scales as $Re^{3/4}$, so the mesh size must be increased by ~180x in each direction
- Compute power required for a single time step calculation at industrial scale increases by 5,600,000x… to 225 PetaFLOPS!

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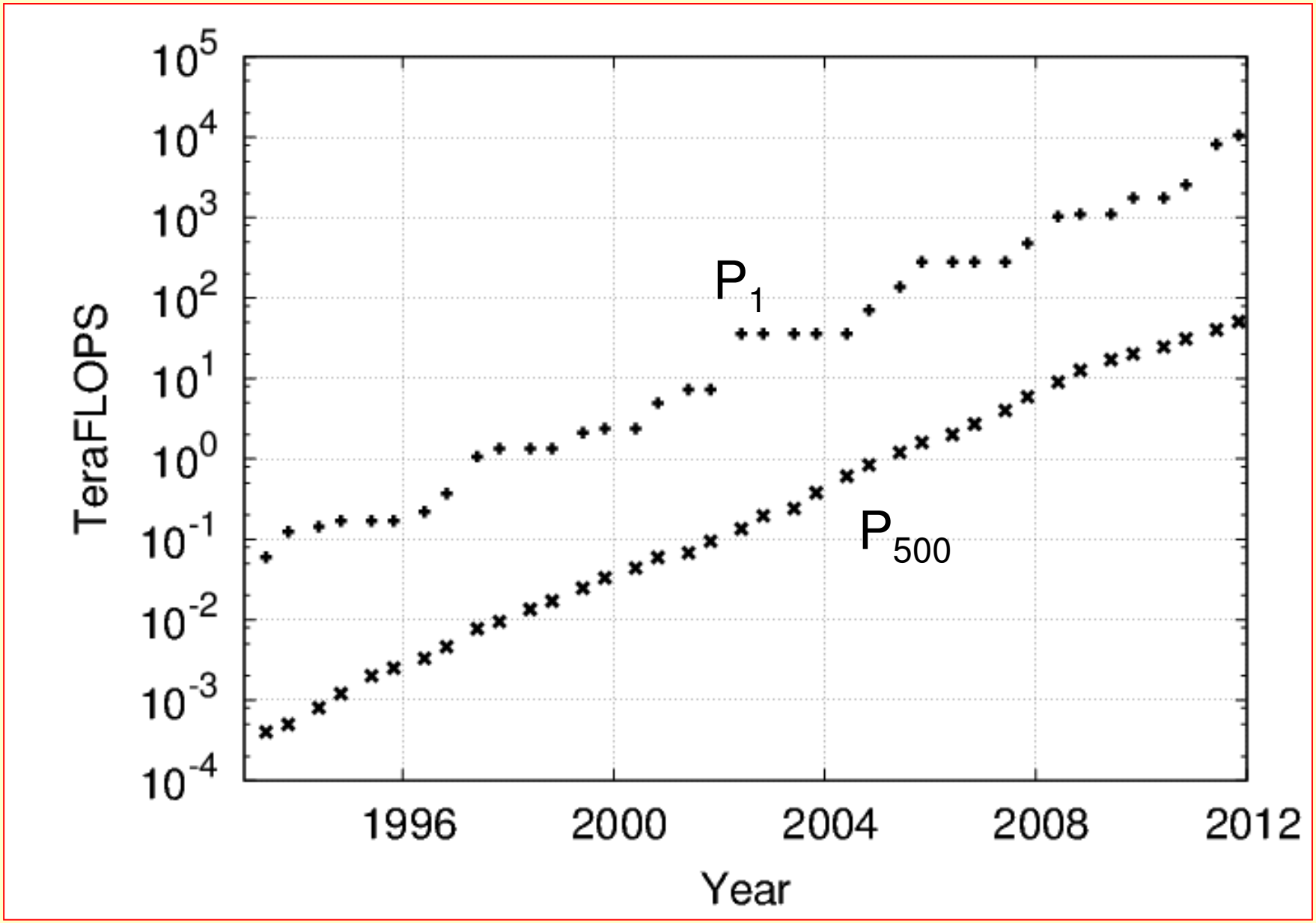
Computing Resources – Top500 List



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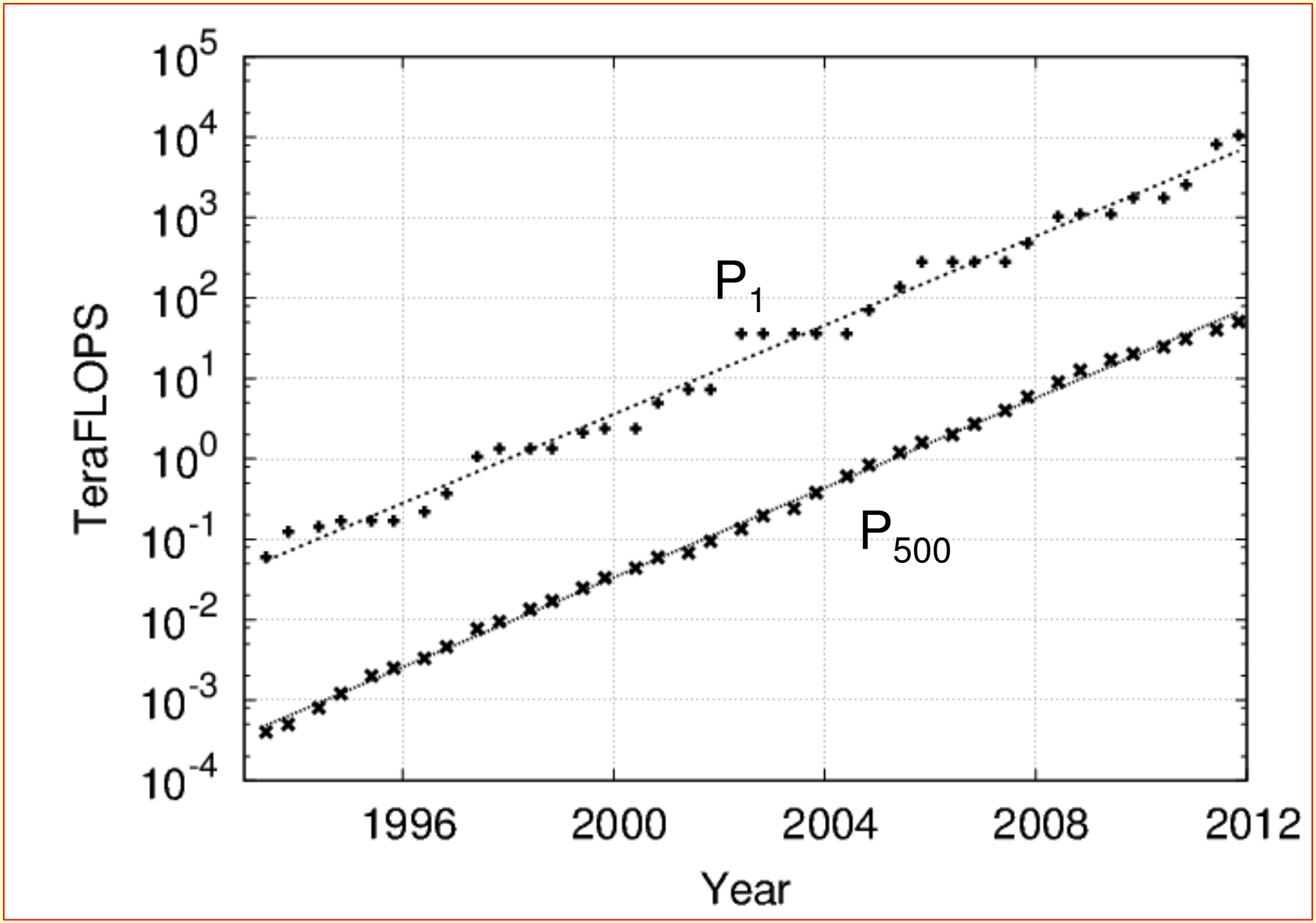
Computing Resources – Top500 List



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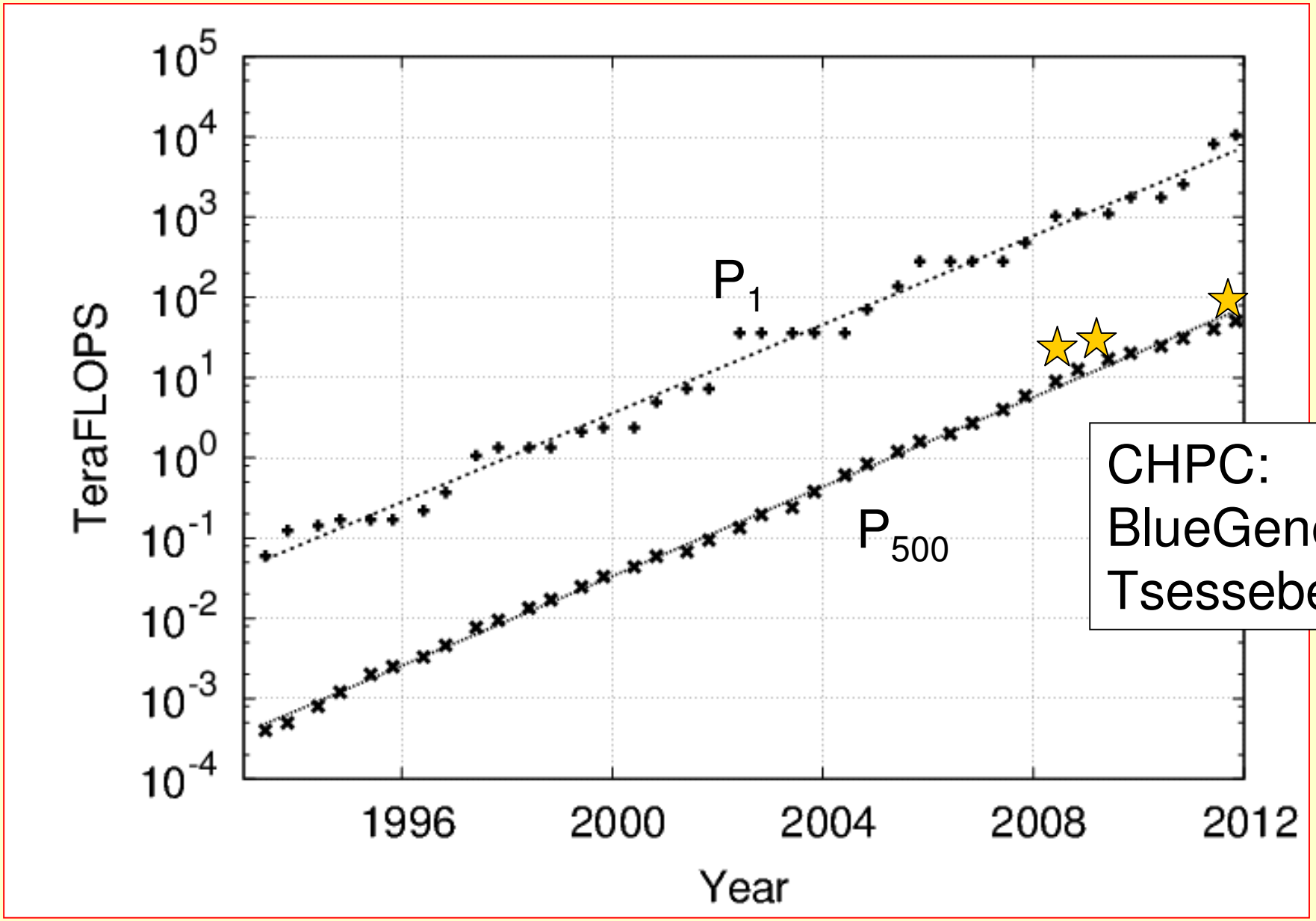
Computing Resources – Top500 List



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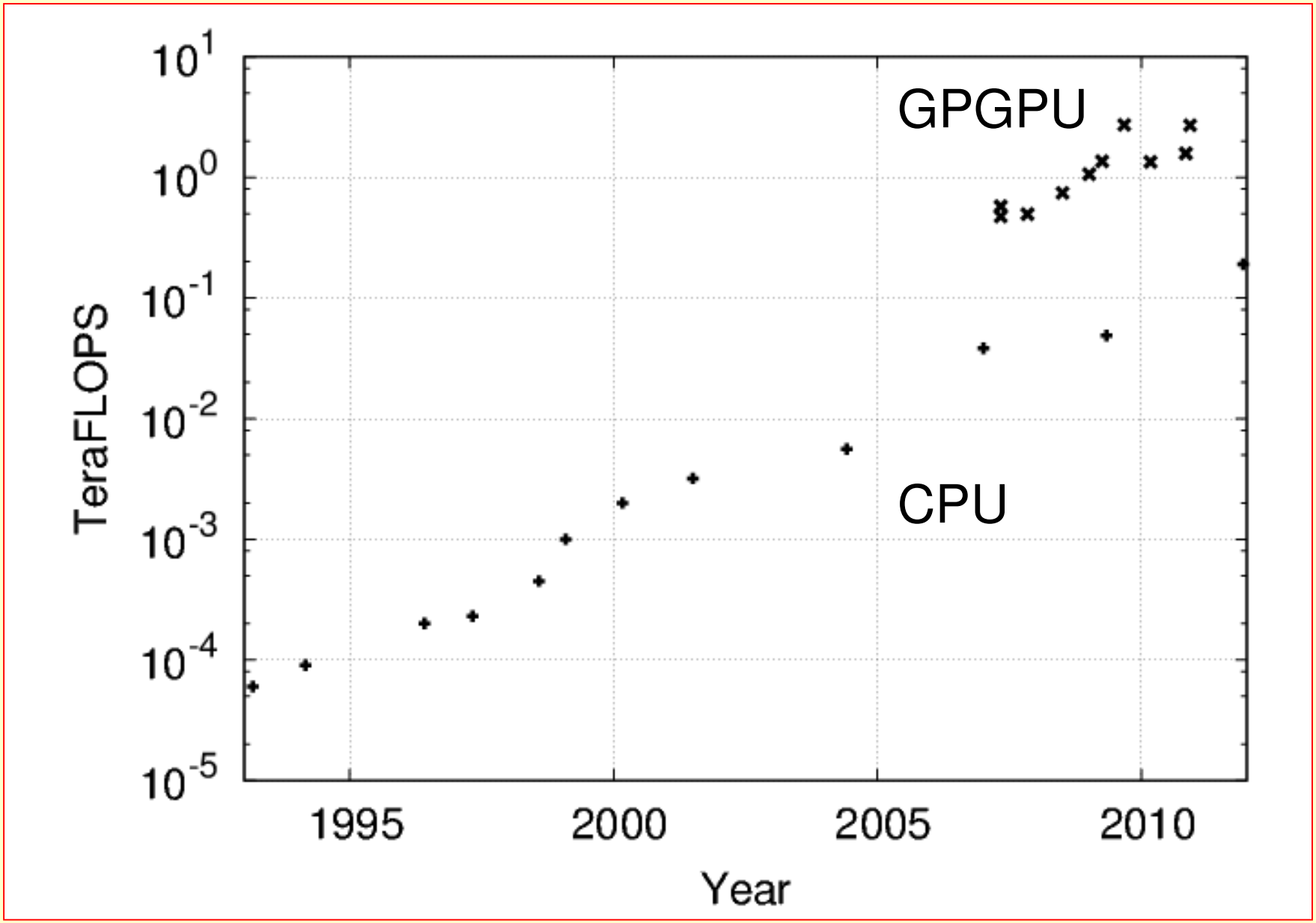
Computing Resources - Desktop



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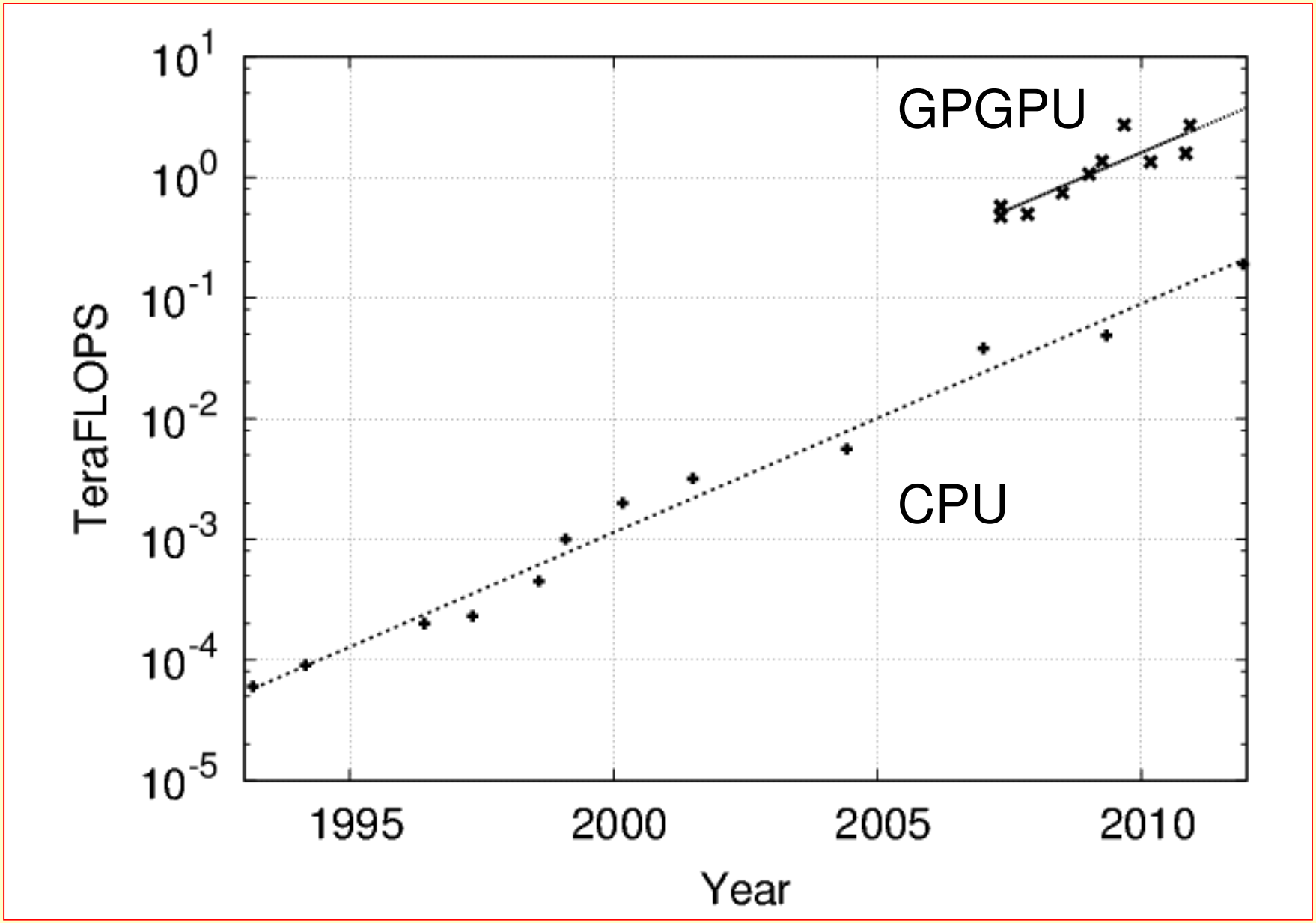
Computing Resources - Desktop



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TeraFLOPS are so last year, man

- Sustained exponential growth in available computing power in all areas
- HPC power grows faster than Desktop power, but disruptive technologies (eg GPGPU) can produce orders-of-magnitude leaps forward
- Massive parallelism and processor/communications heterogeneity is already prevalent in HPC, coming to desktops soon

…

- But to get back to our original question – when are we going to get those 225 PetaFLOPS?

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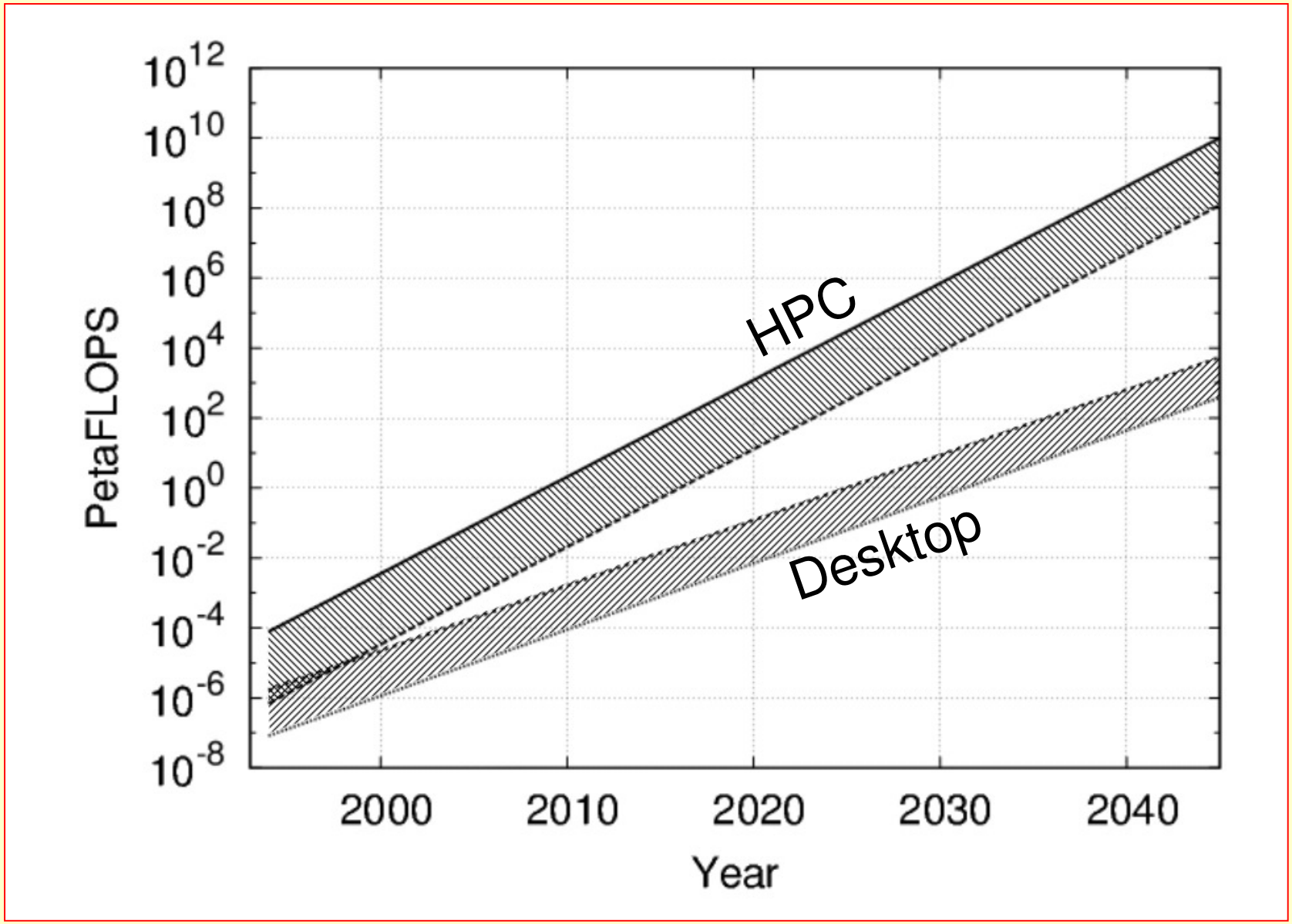
Some Predictions



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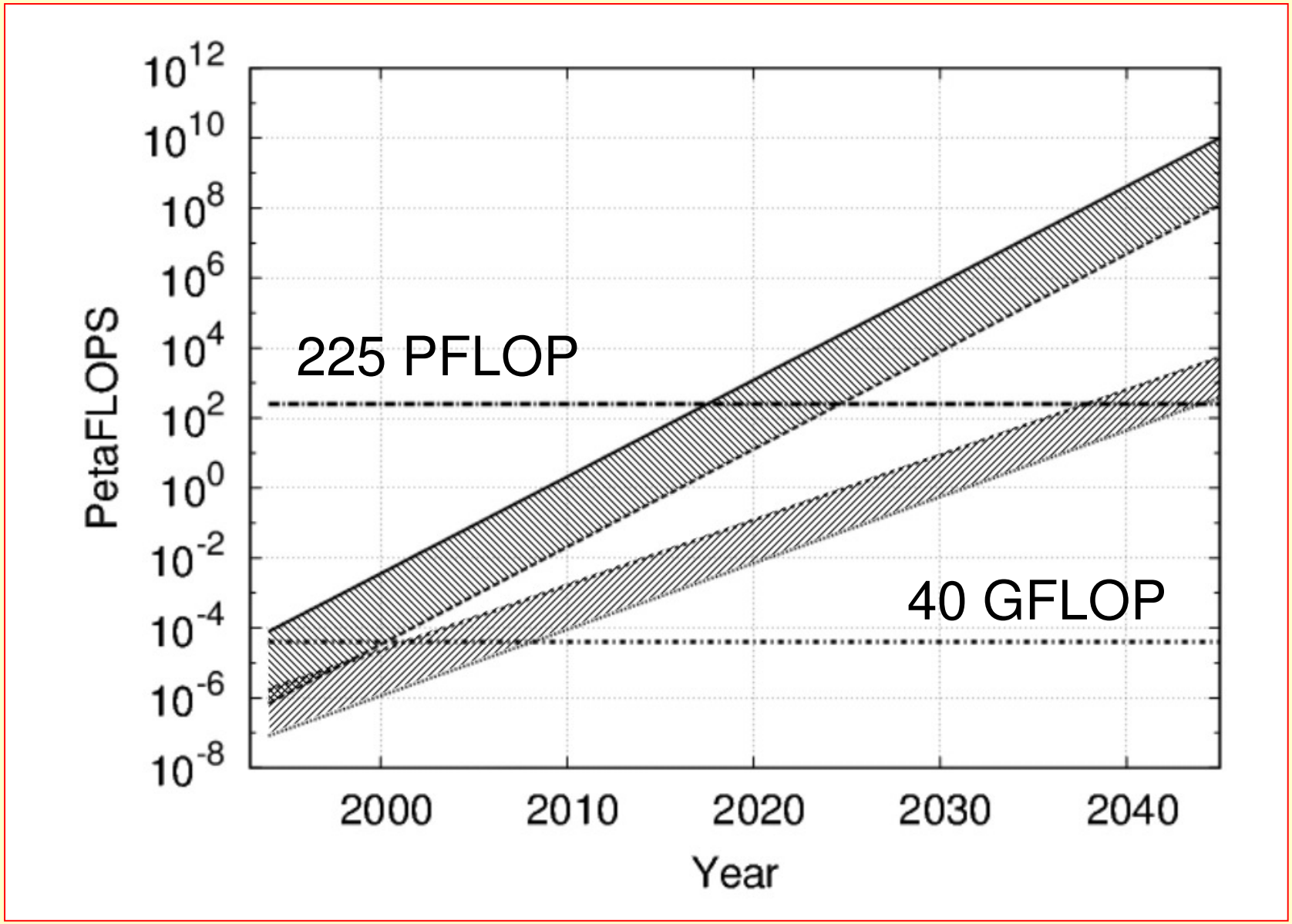
Some Predictions



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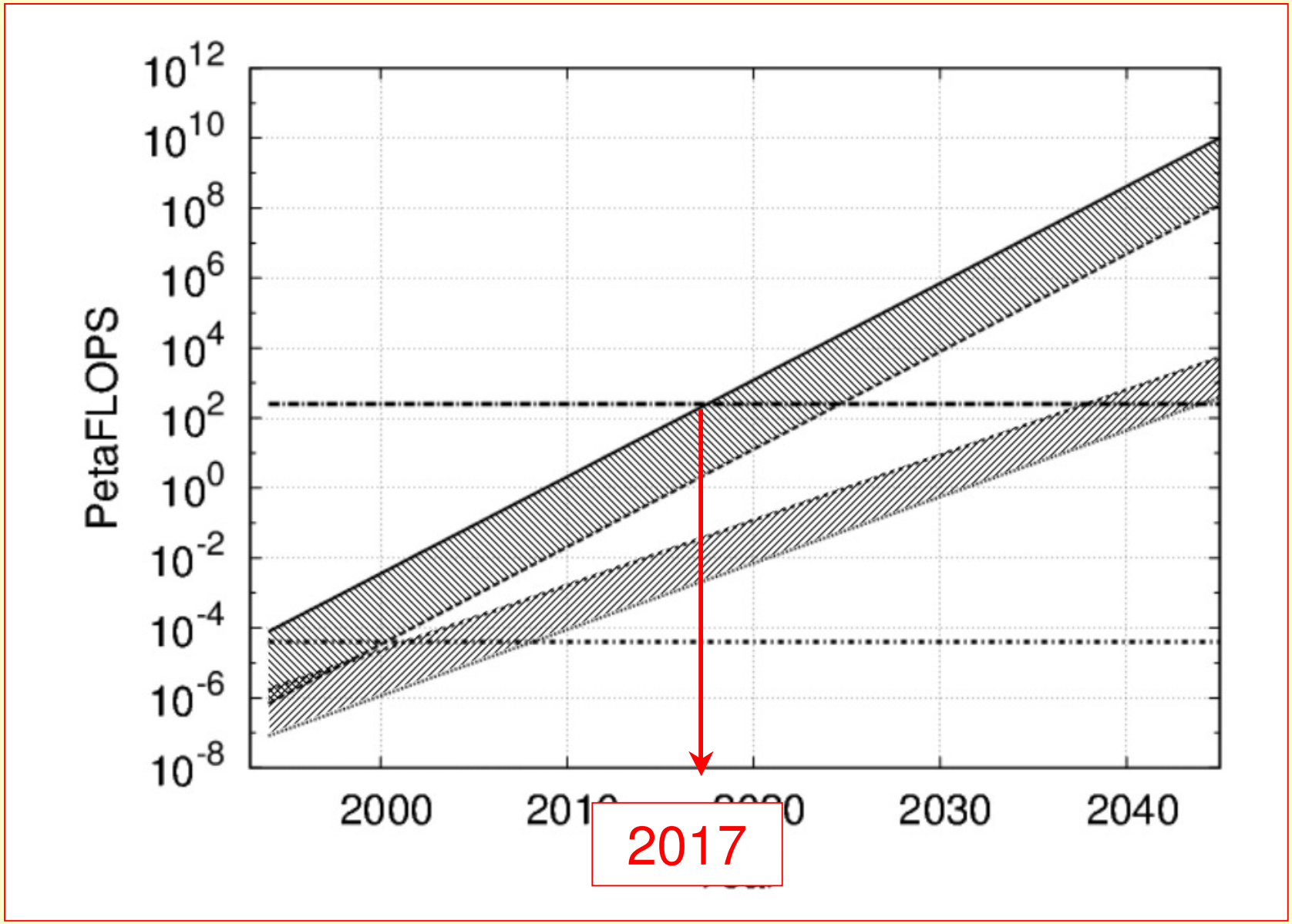
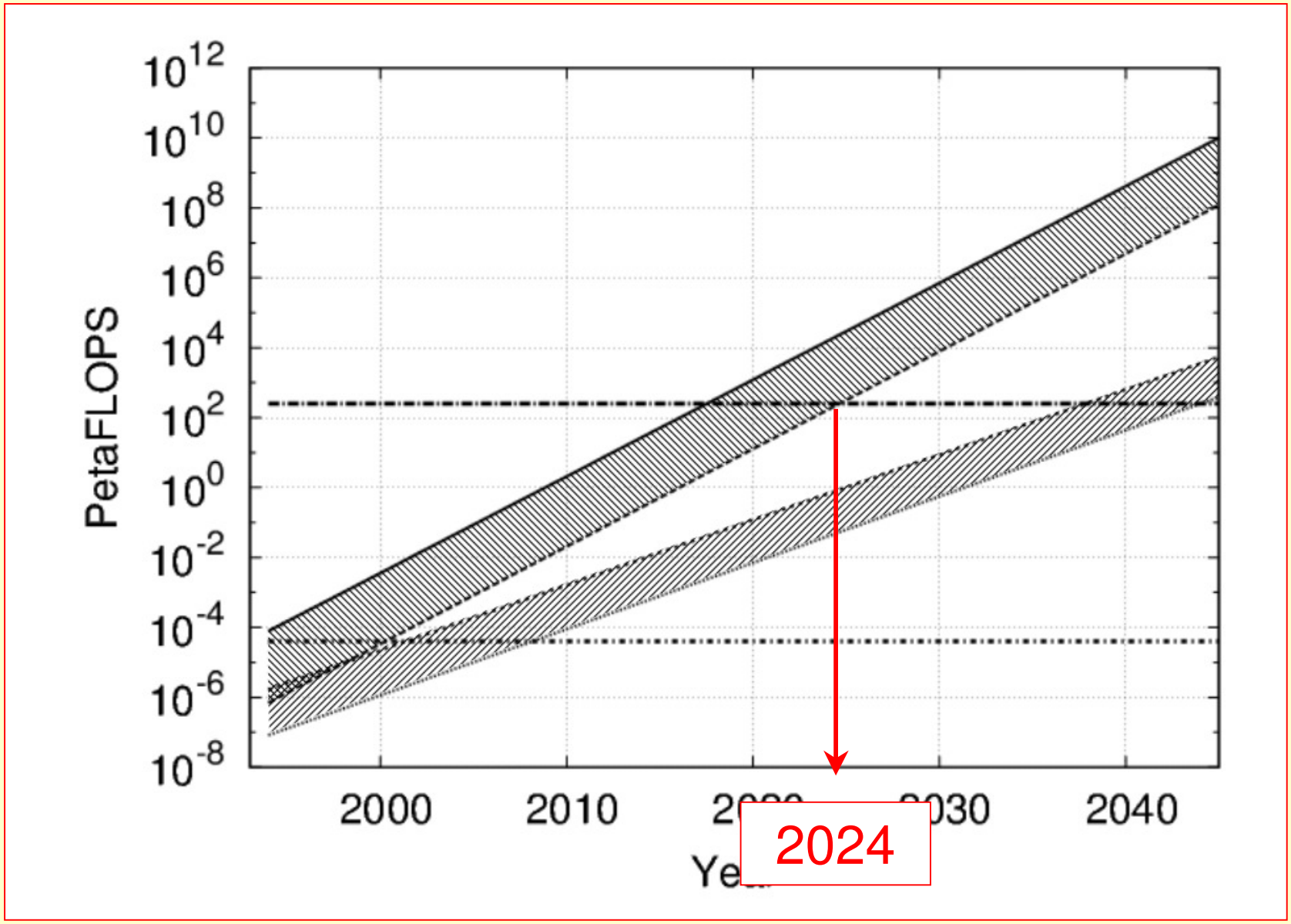
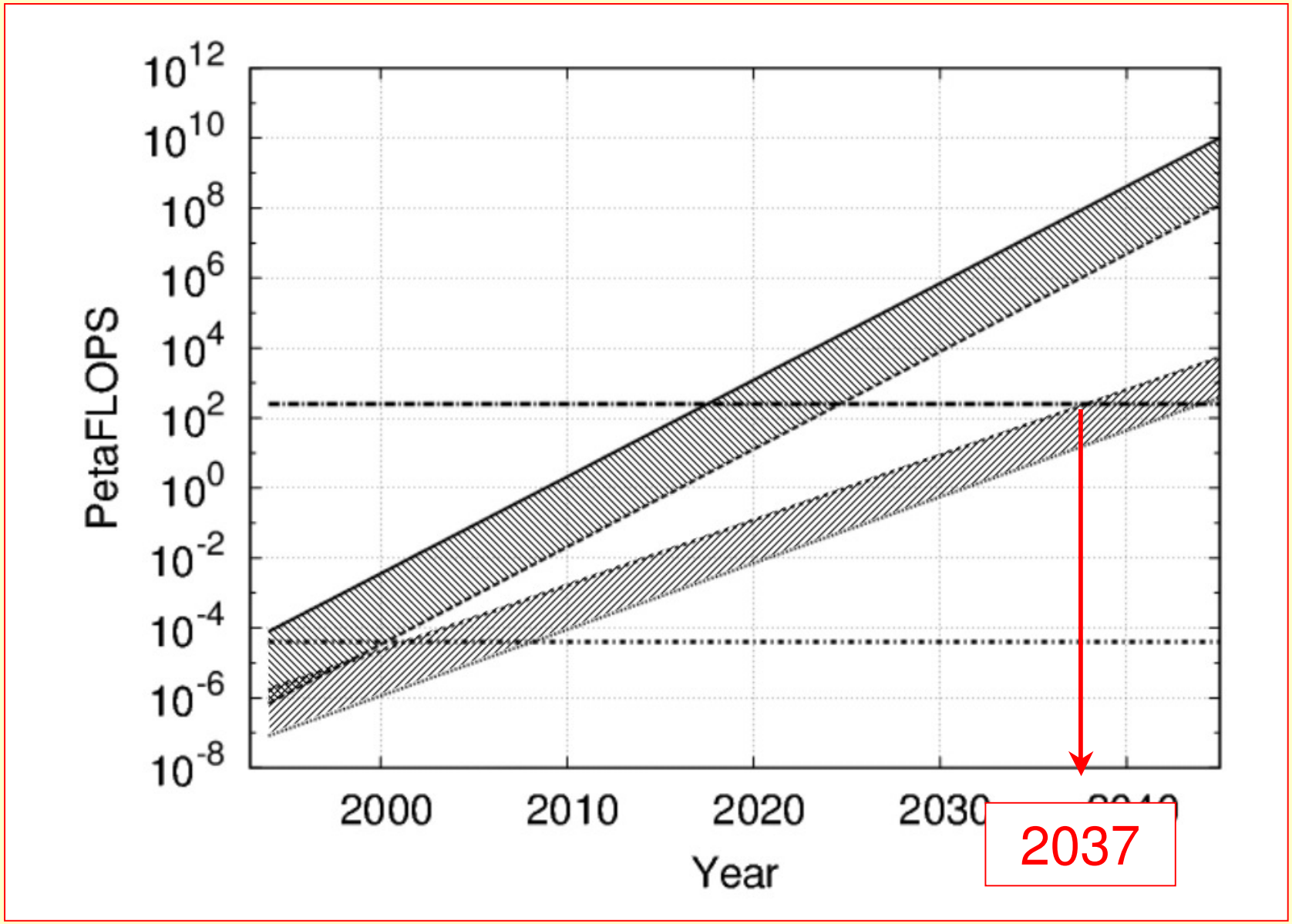
Fastest machine in the world…



Slowest machine on the Top500…



Fastest machine on the desktop…



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The Perfect Storm

- In order for modelling to be widely adopted in any industry, three things are required:
- ***Hardware*** (fast, accessible computers!)
- ***Software and tools*** (clever math and code!)
- ***Expertise and human capital*** (smart people!)

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The Perfect Storm

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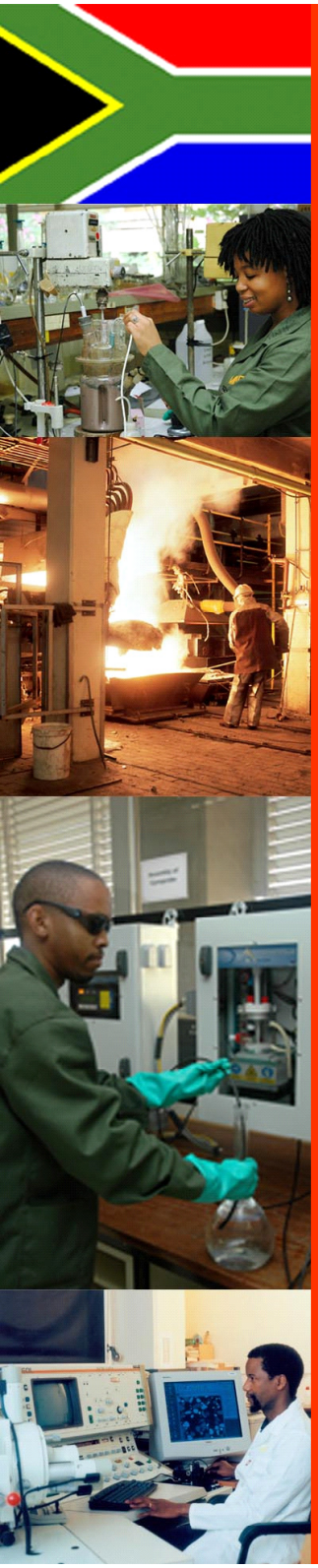
HPC Resources in South Africa

- ***CHPC***
  - Centre for High Performance Computing
- ***SANReN***
  - SA National Research Network
- ***SAGrid***
  - SA National Compute Grid
- ***DIRISA***
  - Data Intensive Research Infrastructure for SA



Thank you

“Computers are incredibly fast, accurate and stupid; humans are incredibly slow, inaccurate and brilliant; together they are powerful beyond imagination”

– Leo Cherne (attrib.)

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