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Exceptional service in the national interest

Sandia National Laboratories

Some Scientific Supercomputing

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Why do we need a supercomputer?

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- Solve problems faster.
- Solve big problems.
- Solve big problems fast enough.
- Perform lots of experiments.

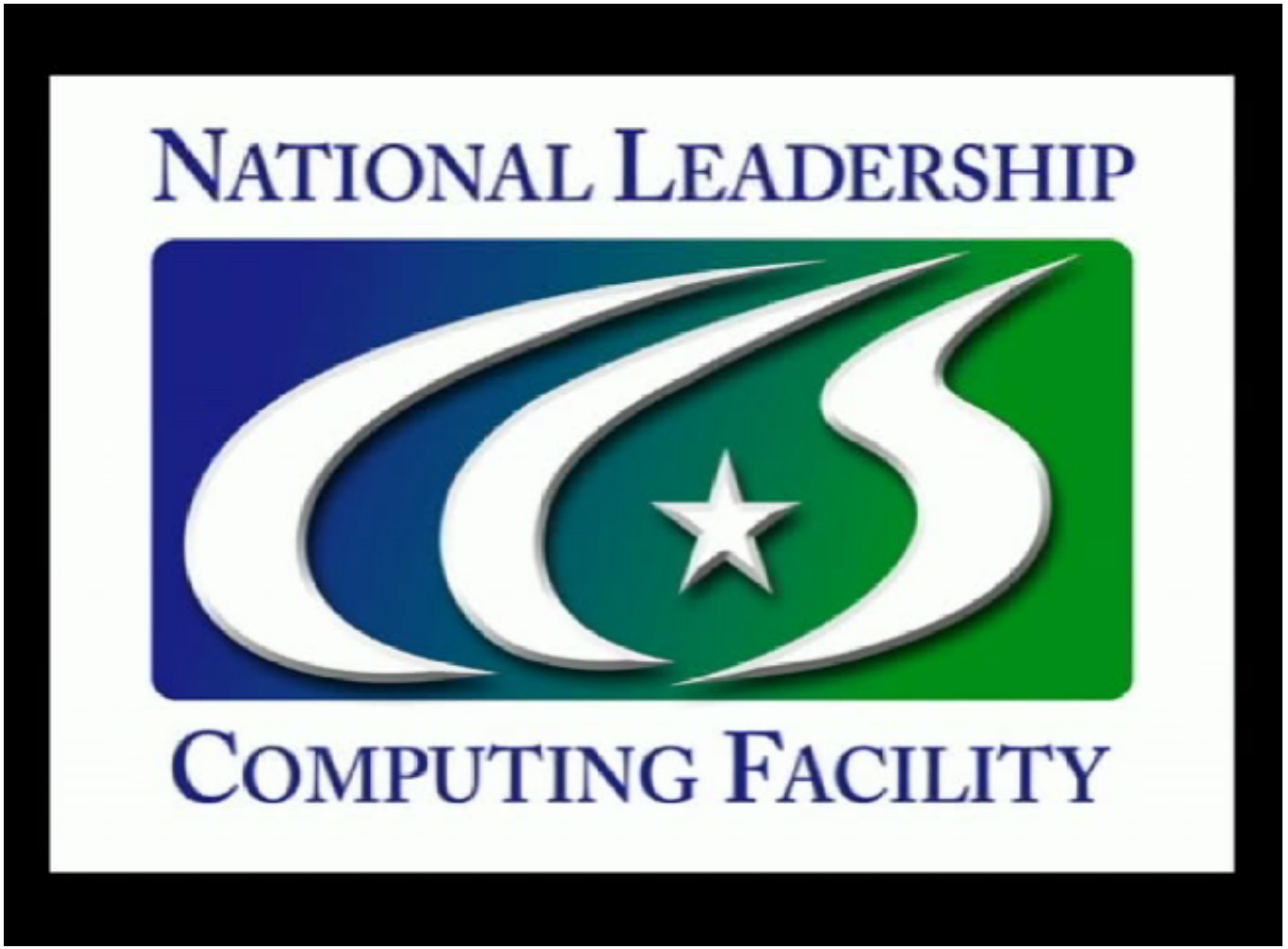
Climate modeling

- Where does “big” come from?
  - Spatial resolution: grid cells every 50km, 30 layers.
    - Temperature, wind velocity, humidity, etc. Times 8 bytes each variable.
- Where does “fast” come from?
  - Lots of work per cell.
  - Time: 30 minute time steps for 100 years = 1,753,152
    - Hundreds of thousands of lines of code.
- “As a general rule, increasing the resolution of a model by a factor of two means about ten times as much computing power will be needed (or that the model will take ten times as long to run on the same computer).” NCAR web site.
- How many experiments do I need to run to reach a conclusion?

Code sketch

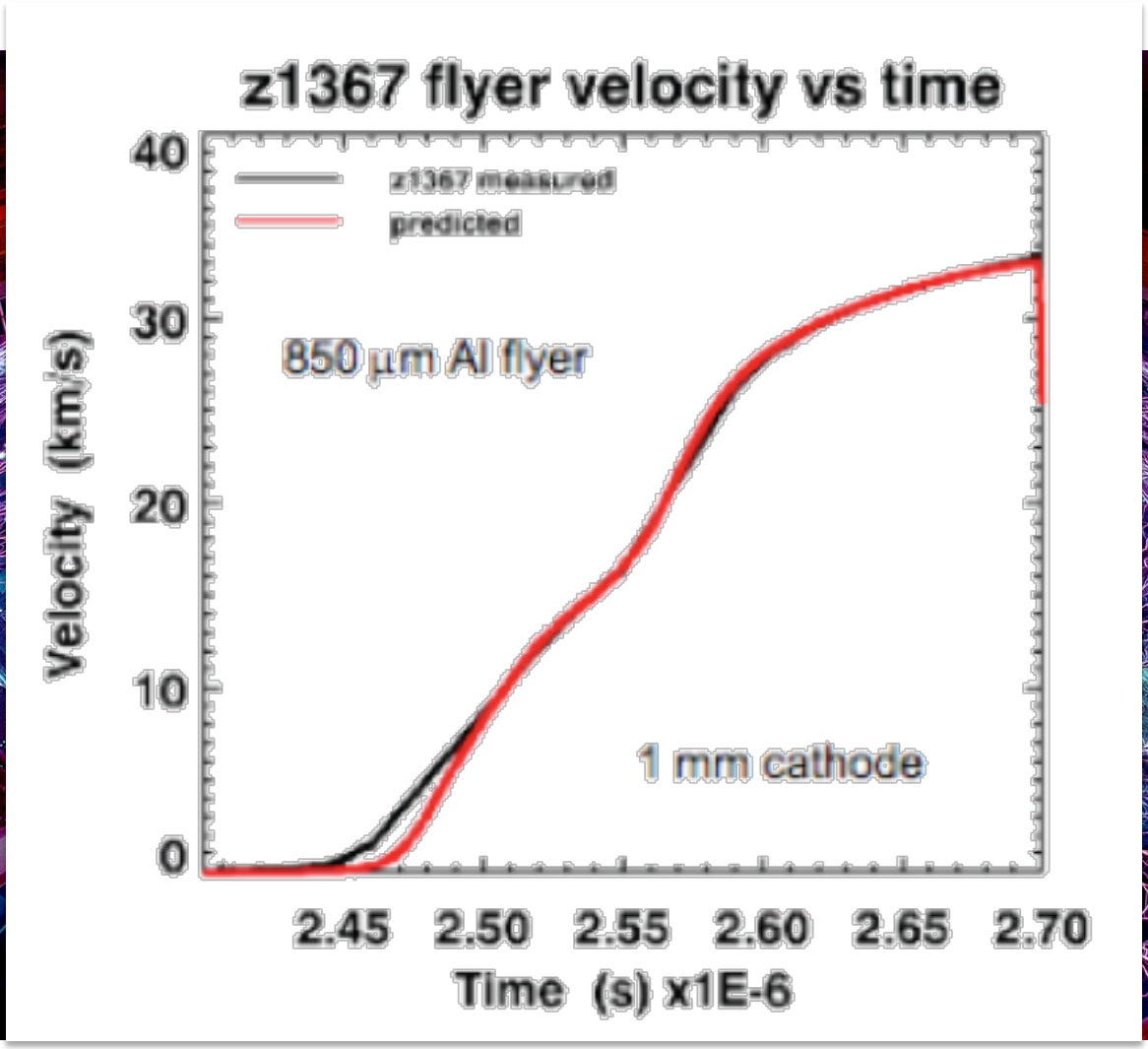
```
ierr = MG_Boundary_exchange ( ... );

ierr = MG_Boundary_conditions ( ... );

ierr = MG_Stencil_3d7pt ( ... );
```

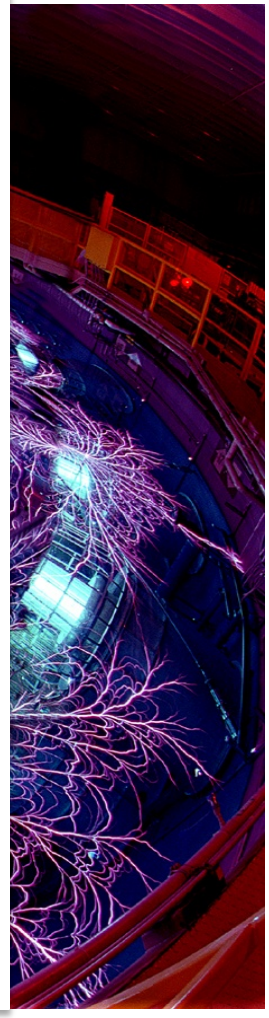
```
for ( k=0; k<=nx; k++ ) {
for ( j=0; j<=ny; j++ ) {
for ( i=0; i<=nz; i++ ) {

   out(i,j,k) = (
                            in(i,j,k-1) +

                        in(i-1,j,k) +
        in(i,j-1,k) + in(i,  j,k) + in(i,j+1,k) +
                        in(i+1,j,k) +

                    in(i,j,k+1)
     )

     / SEVEN;
```

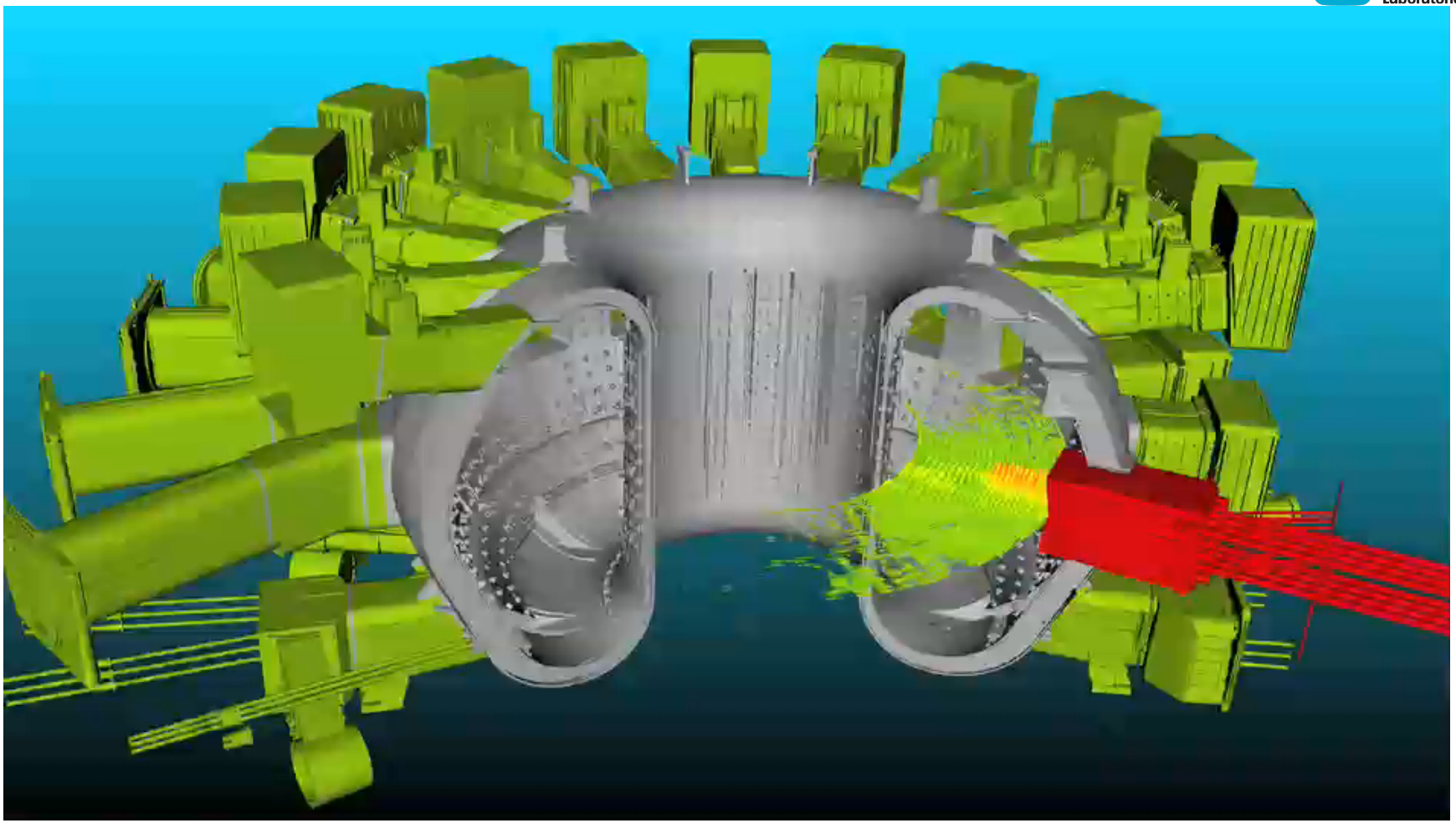

NATIONAL LEADERSHIP
COMPUTING FACILITY

- https://www.youtube.com/watch?v=TVaIvAPMd_g

Configuring the Z-machine using ALEGRA







Shown on History Channel "Modern Marvels" show "Super Hot"

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Fusion energy

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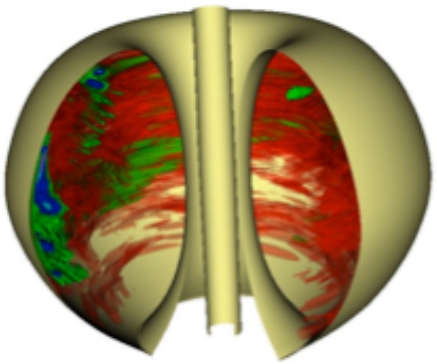
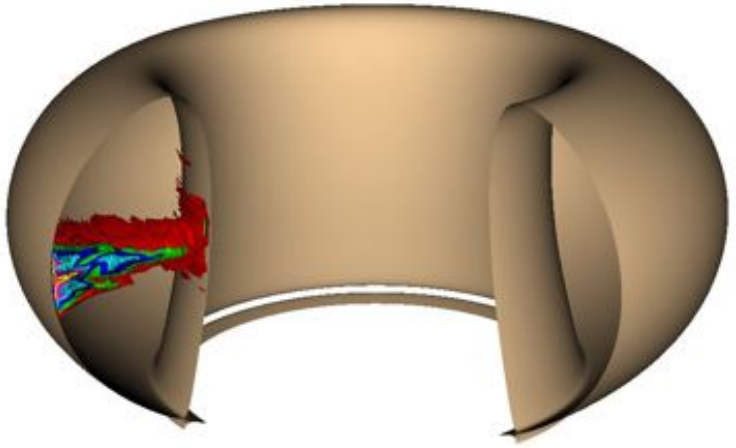
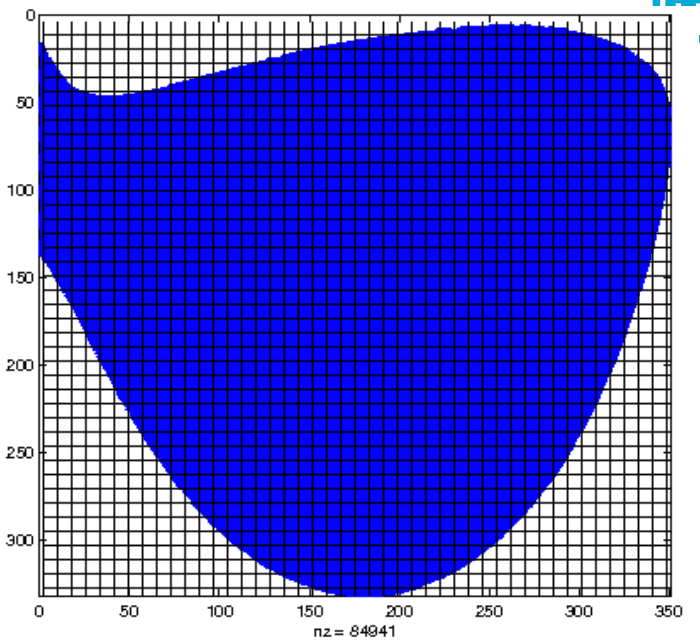




Fusion energy

2d slice of the cavity



Each grid point a dense linear equation of complex coefficients (@16 bytes).

512 x 512 => 262k equations: Ax = b
(~1 Tbyte)

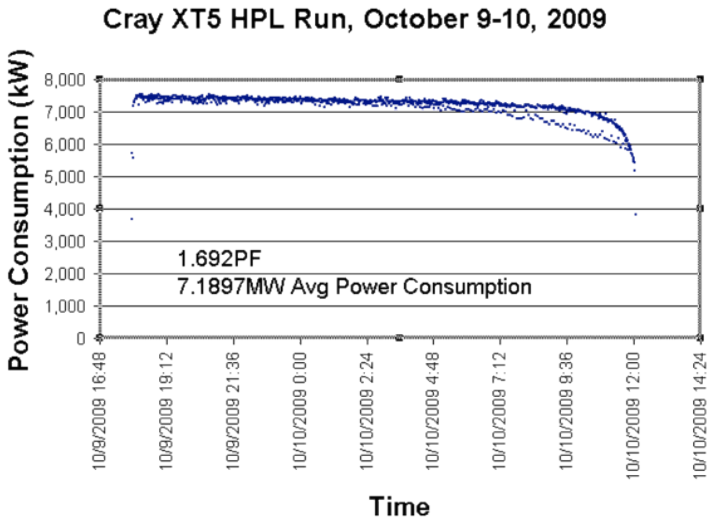
For N equations, work is

$$2/3\ N^3 + 2\ N^2 + O(N).$$

For an accuracy of

$$< \frac{\| Ax - b \|_\infty}{\|A\|_\infty \|b\|_\infty\ n\ \varepsilon}$$

Order hours of runtime each iteration.



Computing capabilities inspires new algorithms

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- Linear solvers
- Monte Carlo