# Advances in Modeling the Generation of the Geomagnetic Field by the Use of Massively Parallel Computers and Profound Optimization


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# The Geomagnetic Field

**At the Earth's surface, the magnetic field that is observed is similar to that that would be generated by a simple bar magnet running through the Earth's axis.**

- This idea (permanent magnetism) was commonly believed a century ago.
- Because the temperature of the core is so high, permanent magnetism is not possible.
- Therefore, the magnetic field should decay, over tens of thousands of years.
- Since it does not, the field must be regenerating.
- Since the turn of the century, the idea that the core is molten iron which by moving generates a magnetic field arose.
- The set of equations to describe this are extremely non-linear and complex.
- Only in the last five to ten years have computers been able to solve these equations.

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## Geomagnetic Equations

$$\rho = \left[ \left( \frac{\partial \overline{\rho}}{\partial S} \right)_{\xi,p} S + \left( \frac{\partial \overline{\rho}}{\partial \xi} \right)_{S,p} \xi + \left( \frac{\partial \overline{\rho}}{\partial p} \right)_{S,\xi} p \right]$$

Equation of State

$$\nabla \cdot \overline{\rho} \mathrm{v} = 0$$

Mass Conservation

$$\nabla \cdot \mathrm{B} = 0$$

Magnetic Flux Conservation

$$\nabla^2 U = 4\pi G \rho$$

Gravitational Potential

$$\frac{\partial \mathrm{B}}{\partial t} = \nabla \times (\mathrm{v} \times \mathrm{B}) - \nabla \times (\overline{\eta} \nabla \times \mathrm{B})$$

Magnetic Induction Equation

$$\overline{\rho} \frac{\partial \mathrm{v}}{\partial t} = -\nabla \cdot (\overline{\rho}\, \mathrm{vv}) - \overline{\rho} \nabla (p / \overline{\rho} + U) - \left[ \left( \frac{\partial \overline{\rho}}{\partial S} \right)_{\xi,p} S + \left( \frac{\partial \overline{\rho}}{\partial \xi} \right)_{S,p} \xi \right] \overline{g} \hat{r}$$
$$+ 2\overline{\rho}\, \mathrm{v} \times \Omega + \nabla \cdot \left( 2\overline{\rho}\overline{\nu} \left( \vec{\vec{e}} - \frac{1}{3} (\nabla \cdot \mathrm{v}) \vec{\vec{\delta}} \right) \right) + \frac{1}{\mu_0} (\nabla \times \mathrm{B}) \times \mathrm{B}$$

Momentum Equation

$$\overline{\rho} \frac{\partial S}{\partial t} = -\nabla \cdot (\overline{\rho} S\, \mathrm{v}) + \nabla \cdot (\overline{\rho} \overline{\kappa} \nabla S) + \frac{1}{\overline{T} r^2} \frac{d}{dr} \left( r^2 c_p \overline{\rho} \overline{\kappa}^T \frac{d\overline{T}}{dr} \right)$$
$$+ \frac{\overline{\eta}}{\mu_0 \overline{T}} |\nabla \times \mathrm{B}|^2 + \frac{\overline{g}}{\overline{T}} \left[ \overline{\kappa} \left( \frac{\partial \overline{\rho}}{\partial S} \right)_{\xi,p} \frac{\partial S}{\partial r} + \overline{\kappa}^{\xi} \left( \frac{\partial \overline{\rho}}{\partial \xi} \right)_{S,p} \frac{\partial \xi}{\partial r} \right]$$

Heat Equation

$$\overline{\rho} \frac{\partial \xi}{\partial t} = -\nabla \cdot (\overline{\rho} \xi\, \mathrm{v}) + \nabla \cdot (\overline{\rho} \overline{\kappa}^{\xi} \nabla \xi)$$

Compositional Equation

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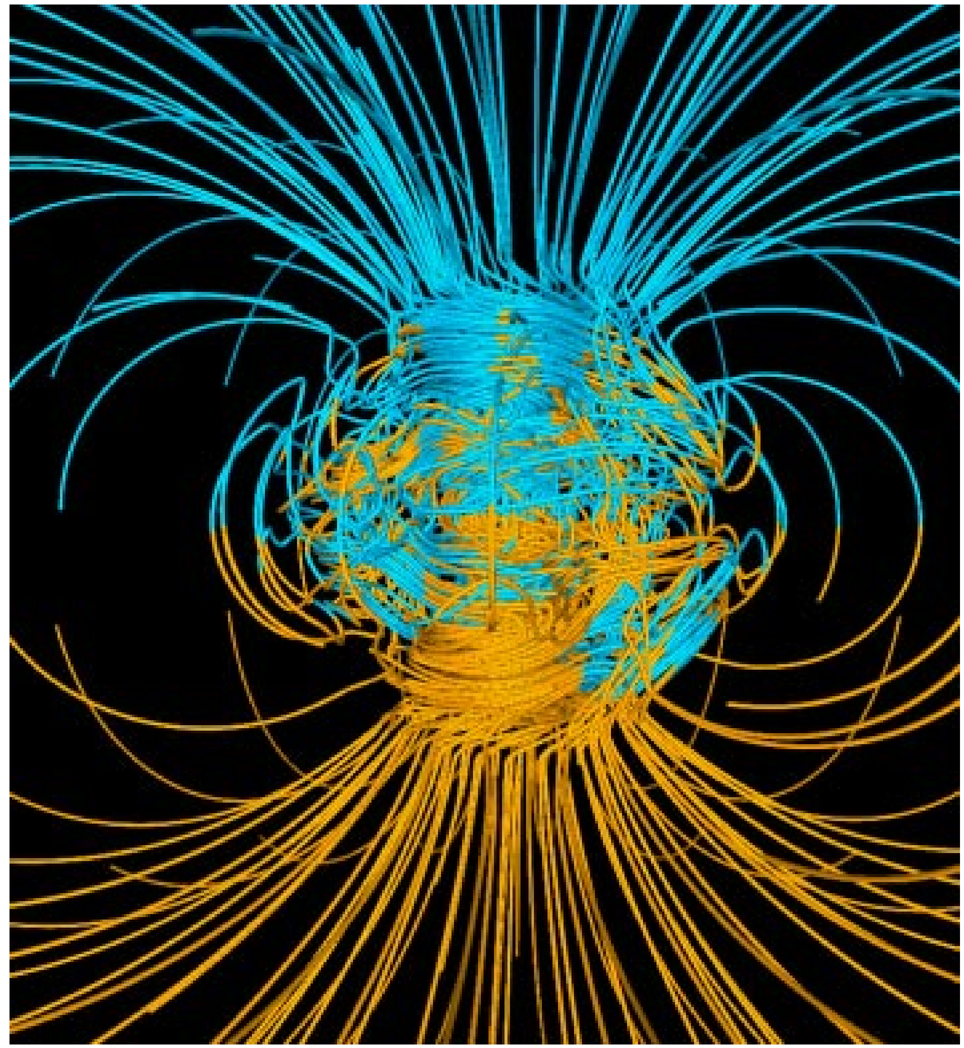
## Magnetic Field Lines



Blue lines are directed inward

Gold lines are directed outward

(Graphic generated by DYNAMO)

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# DYNAMO Code

**Development from 1981 to present by Gary Glatzmaier**

- Based initially on a solar convection code

**Spectral transform method**

- All variables are expanded in spherical harmonics for horizontal structure
- Causes decoupling of spherical degree and order components of variables
- Avoids the pole problem
- Products are computed in grid space

  *Using Fourier and Legendre transforms*

**For small problems, this leads to high accuracy with low cost**

**For large problems, Legendre transforms are an increasing part of the work**

- On parallel machines, they can be done very quickly

**Historically, spectral codes were expected to be poor performers on MPPs**

- Global communication pattern requires every node to communicate with every other node at every time step

# Results of DYNAMO runs

**Fields have correct amplitude and structure outside the core**

- Agree with measurements on Earth's surface and in space

**Time dependence on the short and long time scales agree with measurements**

- Short time scale: drift of non-dipolar part is westward at correct speed
- Long time scale: magnetic field reversal as seen in paleomagnetic record

**Predicted eastward rotation of inner core with respect to the Earth's surface**

- Seismic analyses now show support for this rotation

# Serial Computational Issues

**As problems grow (increasing the spatial resolution) as O(n), the work in the Legendre transforms grows as $O(n^4)$**

- This is the first place to look for optimizations
- We observe that Legendre transforms can be written as matrix-matrix multiplications, because they are independent of r (radial level)
- This implies that level 3 BLAS can be used
  - *These are vendor optimized*
  - *On most machines, these produce the best performance*
- Further observation: matrix-matrix multiplication can be decomposed into the sum and difference of two smaller matrix-matrix multiplications
  - *Savings is almost a factor of 2*
  - *Perform transforms for both the Northern and Southern hemispheres simultaneously with the same number of operations required for a single hemisphere.*

# More Serial Optimization Issues

**Azimuthal transform is FFT, while radial is Chebyshev transforms**

- Both can use vendor-supplied FFT libraries

  *Good performance is likely*

**Other operations can also be replaced by vendor-supplied routines**

- In DYNAMO, LU decomposition is an example

**Ensuring cache friendly coding**

- Use stride 1 references
- Reorder loops so that inner loop varies most quickly
- DYNAMO did not require many changes

**Instead of transforming the entire set of fields to grid space at once, only small subset of the spatial domain are computed at any one time.**

- This is both cache- and memory-friendly

# Parallel Implementation

**Major operations are done locally on each processor, using global transposes to rearrange data as needed**

- Legendre transforms (co-latitude and spherical harmonic degree are local)
- Chebyshev transforms and implicit solves (radius and Chebyshev degree are local)
- Fourier transform (azimuthal wave number and longitude are local)

**The two remaining dimensions are both decomposed over the processors**

- This allows more processors to be used on any given problem size than if the decomposition was just over one remaining dimension

**For the implicit solves, the method of decomposing the two remaining dimensions (spherical harmonic degree and azimuthal wave number) is very important for performance**

- A judicious arrangement of data distribution exists which allows good cache reuse (the matrices can operate on several RHSs simultaneously)

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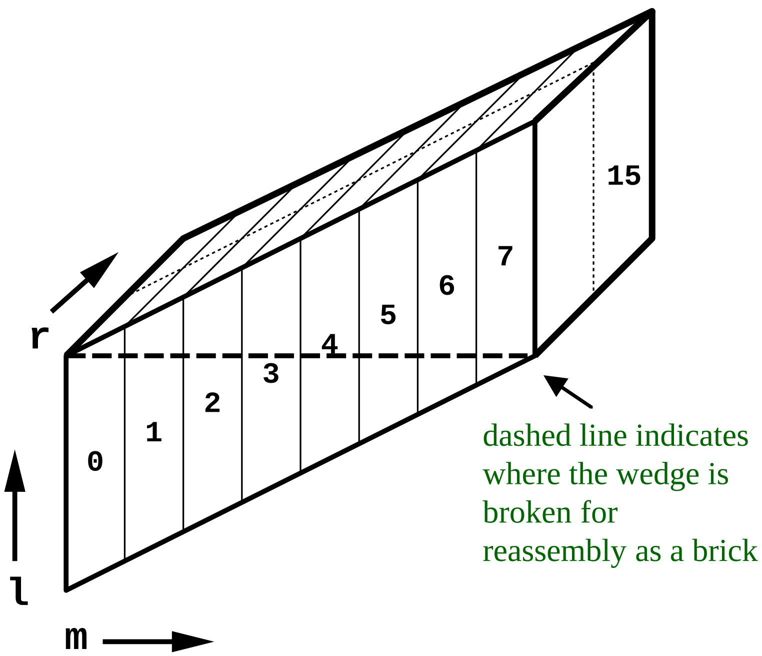
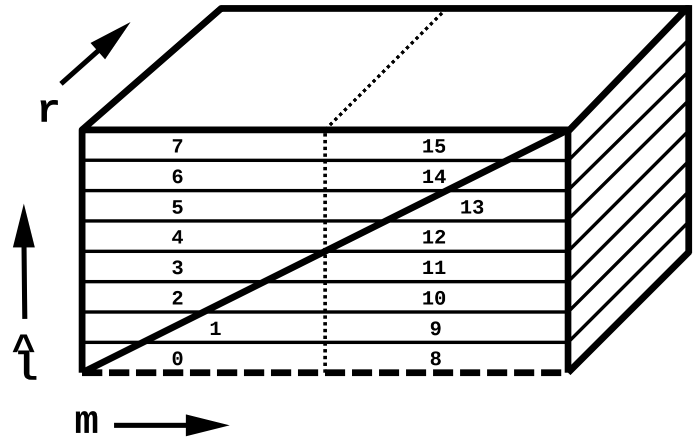
# Data Distribution for Implicit Solves




Data layout used in the spectral domain for Legendre transposes and accumulating linear terms




Data layout used for matrix solves during implicit step

**In addition to performance, this distribution scheme saves memory, since the matrices to be solved depend on l.**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# Cray T3E-Specific Optimizations

**E registers**

- Hardware mechanism that allows processors to directly access memory on remote processors, bypassing the cache
- Can be used for non-unit stride in local memory
- Allows very efficient local transposes

**Shmem libraries**

- Low latency, high bandwidth communications library on T3E
- Requires one-sided calls
- DYNAMO is careful to use long, unit-stride messages
- DYNAMO is careful to schedule communications to avoid hotspots on the network

**Streams**

- Cache pre-fetching mechanism for uniform memory references

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# Performance

**The original code was sequential and could be run on 4 processors of a Cray T90**

- Largest problem that was run: 65 x 150 x 300 (radius x latitude x longitude)
- Overall performance: 1.0 GFLOP/s
- Wall-clock time to solve this problem for 100 years: 24 hours

**The new parallel code has been run on 1488 T3E-1200 processors**

- The largest problem that has been run: 193 x 1858 x 1488
- Overall performance: 637 GFLOP/s
- The wall-clock time to solve this problem for 100 years: 1 year

**Performance improvement: 600 times**

**Wall-clock improvement: 3 times (for the small original problem size)**

*(The current parallel code solves the Coriolis terms explicitly. This dramatically reduces the maximum time step. We are currently testing a new scheme to treat these terms implicitly, which should increase the maximum time step by 50 times.)*

**Most importantly, the maximum possible problem size has increased by 180 times**

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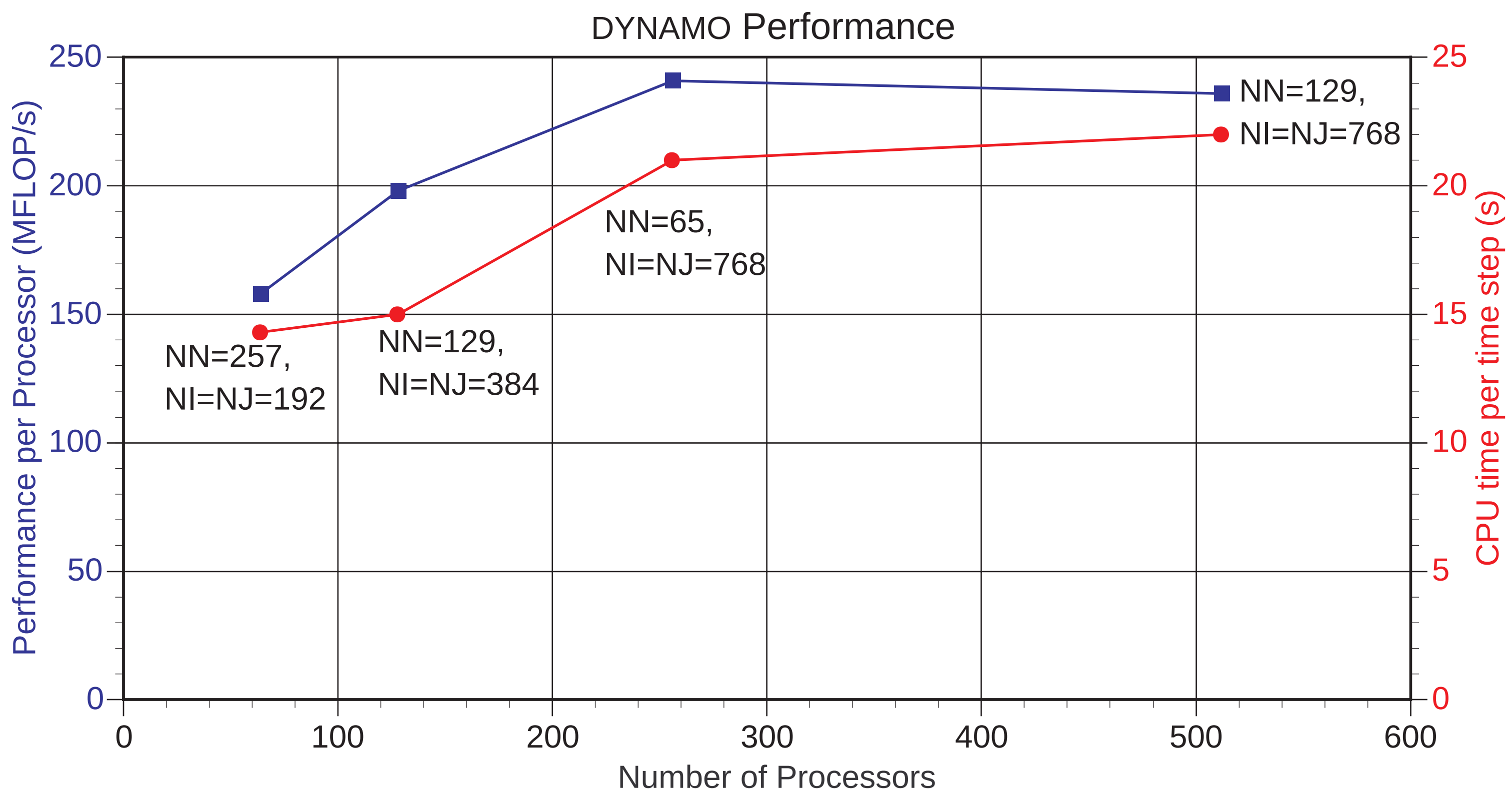
## Scaled-Size Problems




**The problem size is a function of NN*NI*NJ**

**The work is a function of NN*NI*NI*NH**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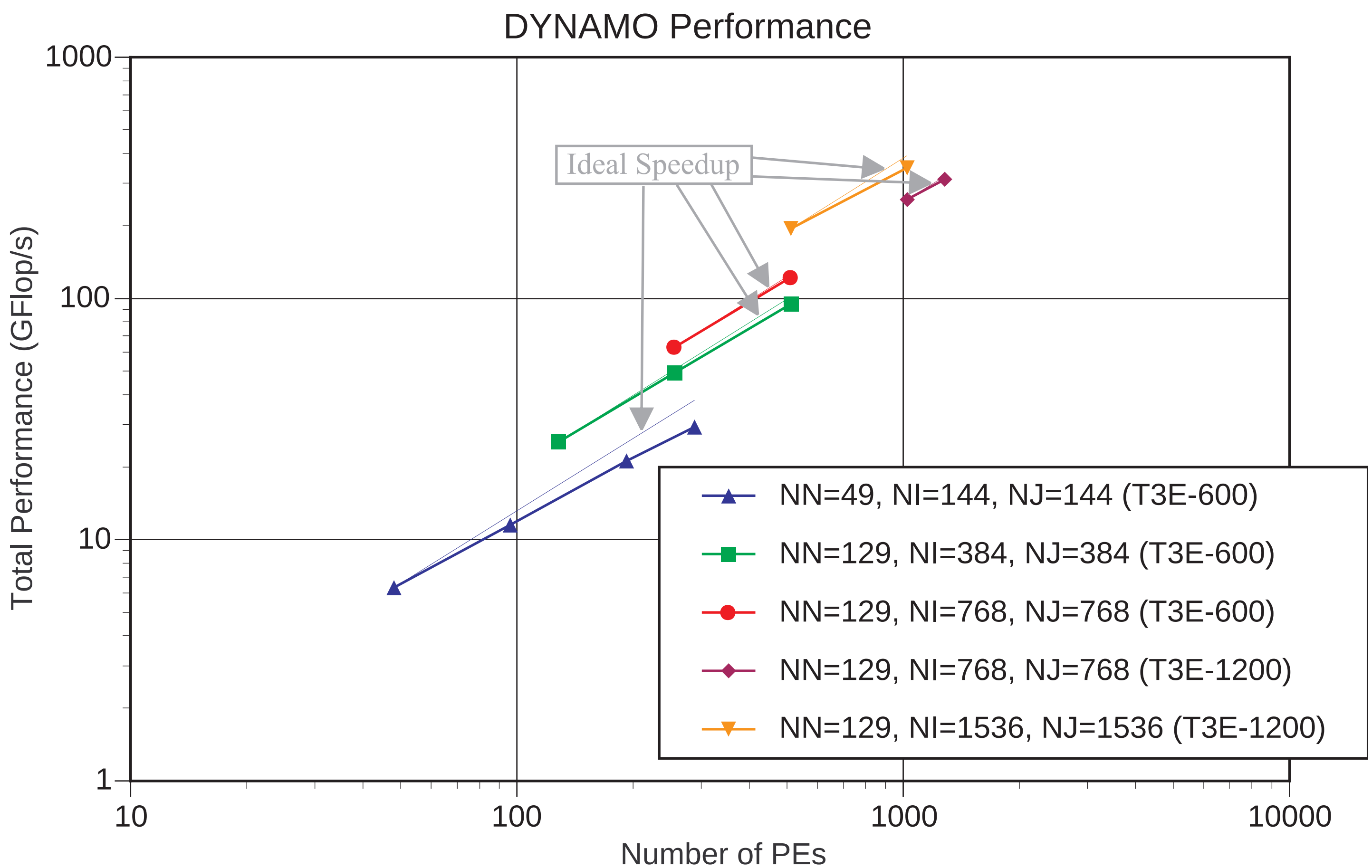
## Fixed-Size Problems

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# Future Work

**Add capability to perform run-time analyses**

- Summarize/Average sections/domains of fields
- Generate animations on-the-fly

**Add MPI switches**

- First, MPI-1 two-sided calls
- Then, MPI-2 one-sided calls

**Port to other machines**

- Origin 2000 is the first target
- Then clusters, SPs, others

**Cleaning-up and documenting the code**

**Pre- and post-processing tools are becoming bottlenecks**

- This is true in many (most?) parallel disciplines

# Conclusions

**On tightly coupled machines, such as the T3E, spectral transform codes work well**

- As problem size increases, relative communications time decreases

**Previous work has been done at lower resolutions**

- Solving for large-scale features has been done by making approximations to eliminate the small-scale details
- This requires material parameters which are known to be non-physical, but do allow computational solution

**High resolution studies will enable new science**

- Smaller-scale features appear
- Realistic material parameters can be used
- An understanding of the required resolution will be obtained, which would provide much more confidence in computational solutions