Fast Algorithms, Potential Theory and Computational Engineering

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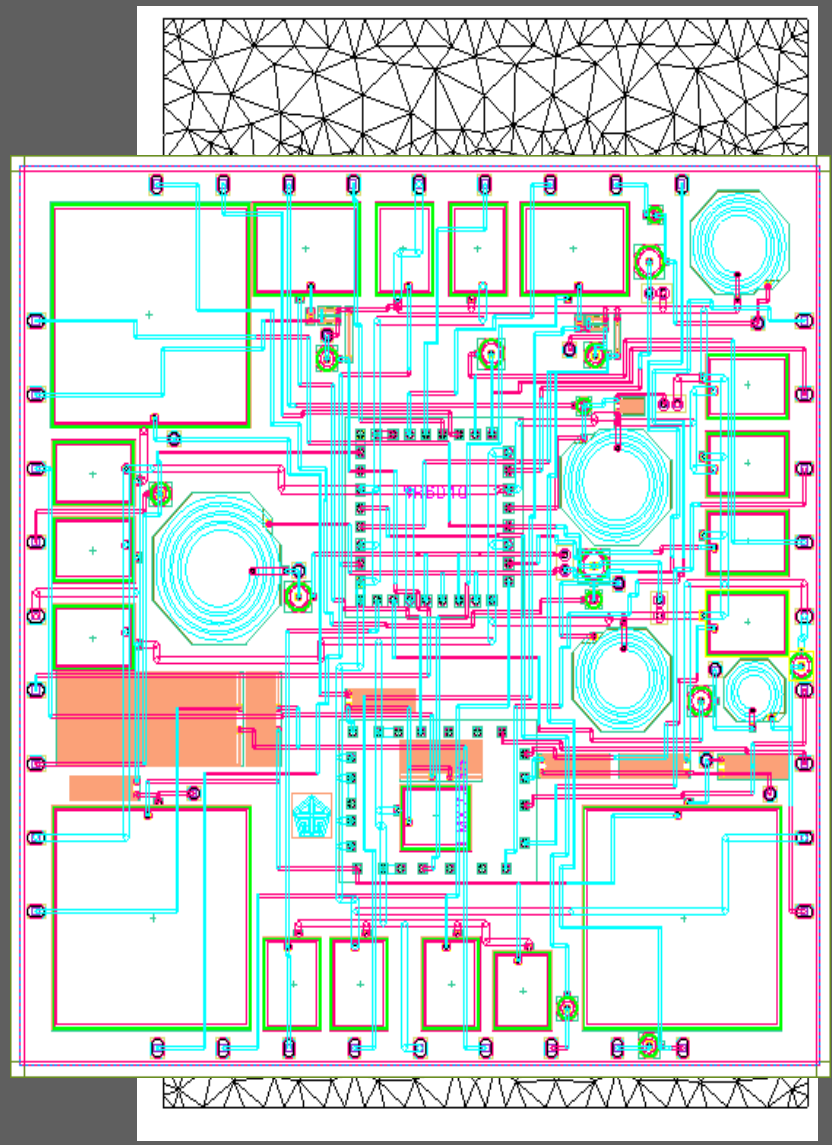
Example

Accurate simulation using traditional techniques is often infeasible

Chip Design, for example, involves both fine-scale features and strong electric field coupling

Efficient solution techniques are essential



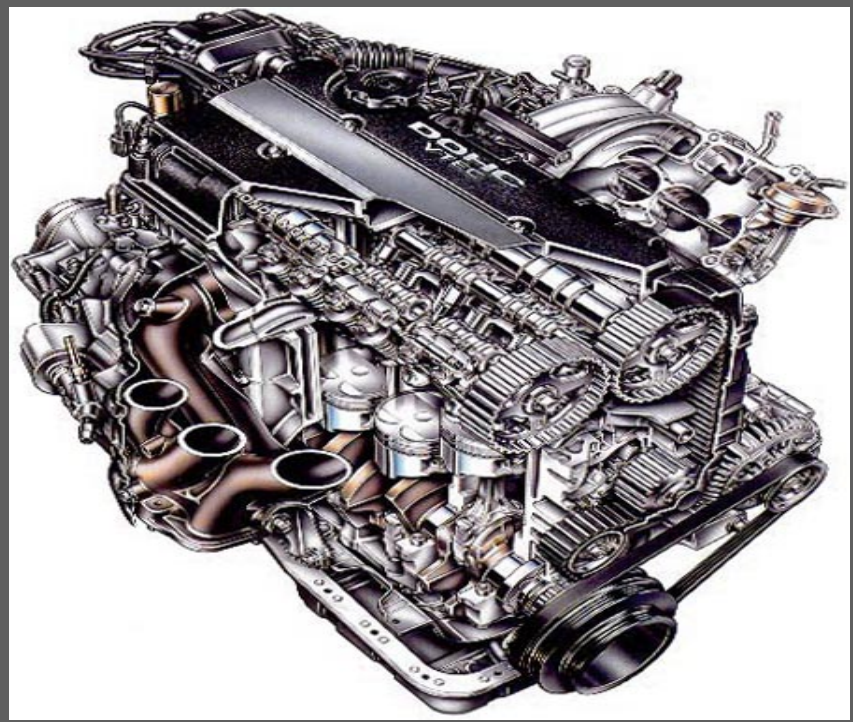
Kapur/Long

Computational Science Issues

- Many of basic methods still in use were developed before WWII.
- People still believe that “the purpose of computing is insight, not numbers” – Hamming (1971). This will not help materials design.
- As machines have gotten faster and faster, the asymptotic complexity of methods has become more and more critical
- The development of modern scientific computing tools is an *engineering discipline* $\Rightarrow$ tables, approximations, tolerances, etc., as well as an underlying *theory*. This requires *judgment*.

Current Environment

- No standards (functionality or performance)
- No support mechanism for low level tools (fuel injectors, starters, batteries, etc.)



Current Environment

- Standard tools for dense linear algebra (LAPACK,MATLAB®)
- Standard tools for small systems of ordinary differential eqs.
- Standard tools for small-scale optimization

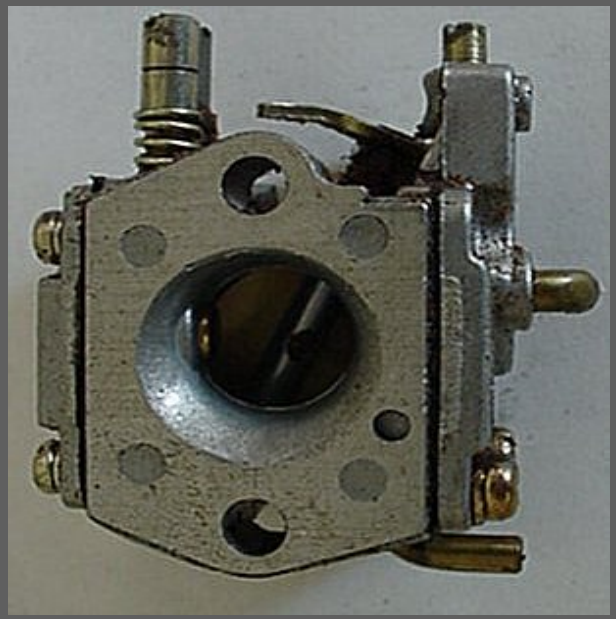
- Slowly being extended (for example) to potential problems:
  - Laplace equation (electrostatics)
  - Helmholtz equation (acoustics)
  - Maxwell equations (electrodynamics)
  - Heat equation (diffusion)
  - Navier-Stokes equations (low to moderate Reynolds number flow)
  - Linear elasticity (MEMS, structural mechanics)

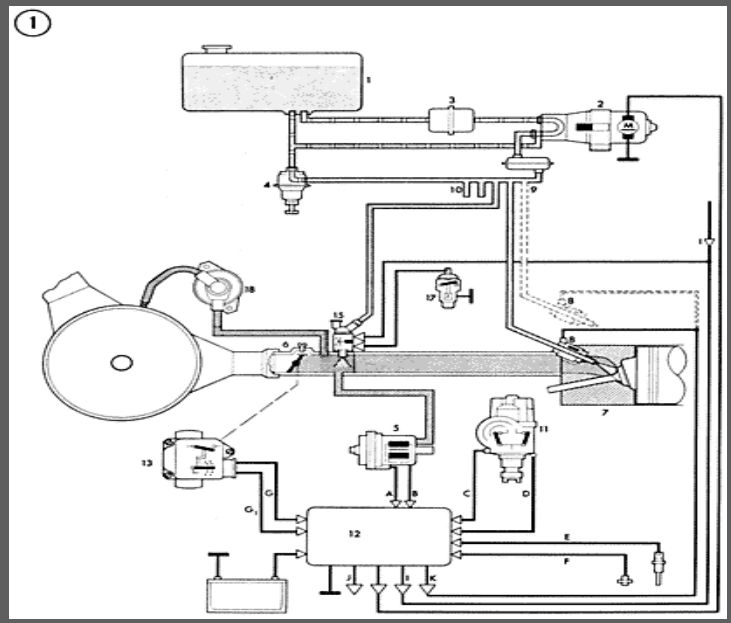
Requirements for modules

- Standardize *problem specification*
- Standardize *testing*
- State *working range of technology* (computational complexity, problem size, available precision, etc.)
- Allow for multiple approaches

- Intermediate level tools are essential for progress (above the dense linear algebra level, below the full application level)

Simple vs. Complex Tools





- Fallacy of “simpler and more general” approaches
- In what sense should tools be flexible?
- Little attention to hierarchy of components

Integral equation methods (Potential theory)

- Ideally suited to many complex problems
- Require fast algorithms to be practical

Integral transforms: $F(x) = \int G(x,y)\, h(y)\, dy$

Integral equations: $h(x) = F(x) + \int G(x,y)\, F(y)\, dy$

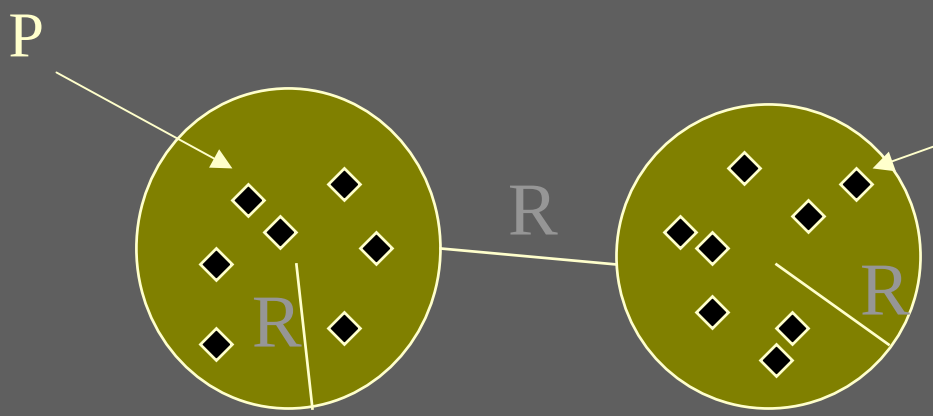
Inverse problems: $h(x) = F(x) + \int G(x,F(y))\, dy$

Kernels of Classical Physics

Diffusion, probability:	$G(r,t) = \exp(- r^2 / t)$
Gravitation, electrostatics:	$G(r) = 1/ r$
Acoustics, Electrodynamics:	$G(r) = \exp(i k r) / r$
Acoustics, Electrodynamics:	$G(r,t) = \delta(r - t)/r$

Black box, fast algorithms now available for all

Electrostatics



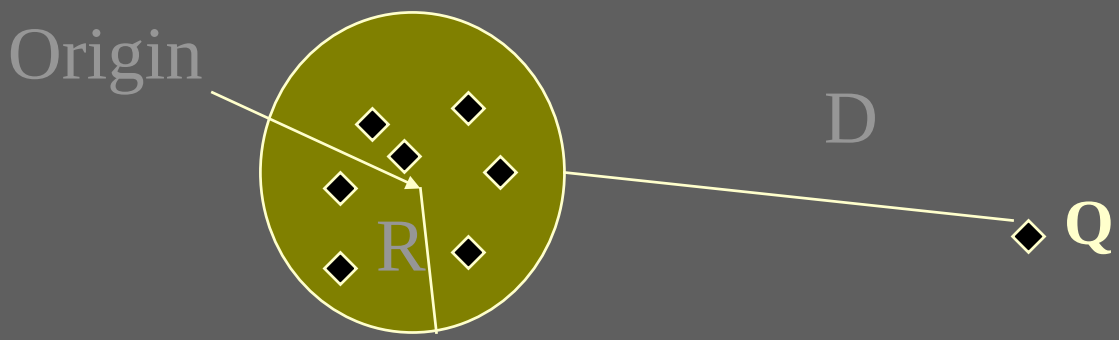
Coulomb interactions

$$V(Q_m) = \sum_{n=1}^{N} S_n / \| Q_m - P_n \|$$

Direct evaluation requires O(N M) work

Fast Multipole Method

(G- and Rokhlin, 1987)

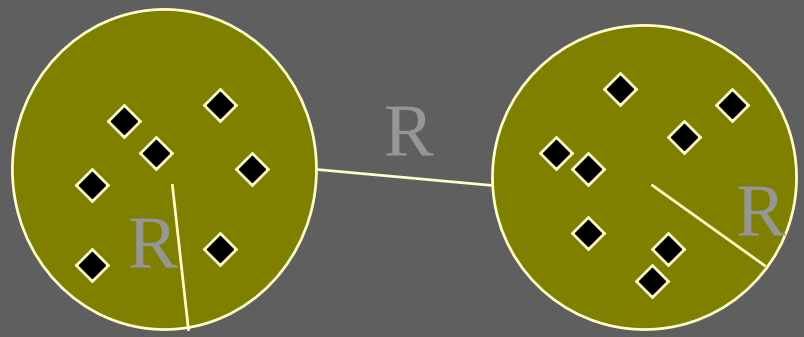


$$V(Q) = \sum_{j=1}^{p} \sum_{k=-j}^{j} M_j^k \quad Y_j^k(\theta, \varphi) / r^{j+1}$$

Error in multipole expansion decays like (R/D)

Setting p = log(ϵ) yields precision ϵ

FMM



1. Evaluate multipole coefficients M_j^k (n = 0,…,p)
2. Evaluate multipole expansion at each target Q_m (m = 1,…,M)

Operation count: O(N+M) rather than O(NM) !

FMM

For more general distributions of sources and targets, the FMM couples previous analysis with a divide & conquer strategy.

- Clustering at various spatial length scales
- Interactions with distant clusters computed by means of multipole expansions
- Interactions with nearby particles computed directly
- Fully adaptive algorithm
- Performance essentially independent of particle distribution

Fast Multipole Methods

N	Lev	p	T_{FMM}	T_{DIR}	Error
500,000	10	10	164	141100	10^{-4}
1,000,000	10	10	282	568100	10^{-4}
500,000	9	19	323	141100	10^{-7}
1,000,000	10	19	714	568100	10^{-7}

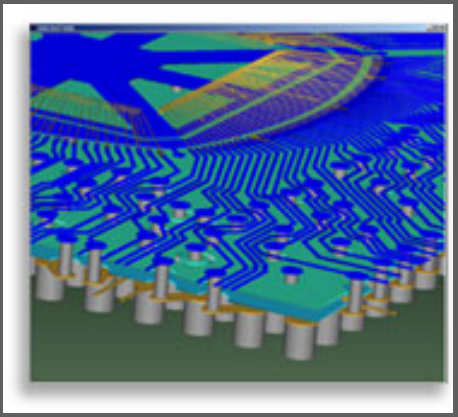
Electrostatic/Electrodynamic/Elastic Interactions with N particles:

Dislocation dynamics (e.g. Wang and LeSar, 1995, …)

Recent parallel implementation (Ying, Biros, Zorin, Harper (2003)

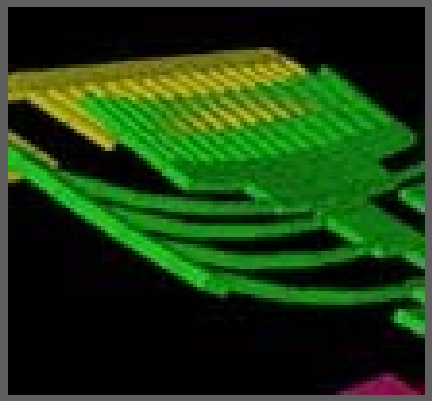
≈1B pts / min

Some Commercial Applications…



ANSOFT TPA™

Automated Signal Integrity Analysis for 3D Packages



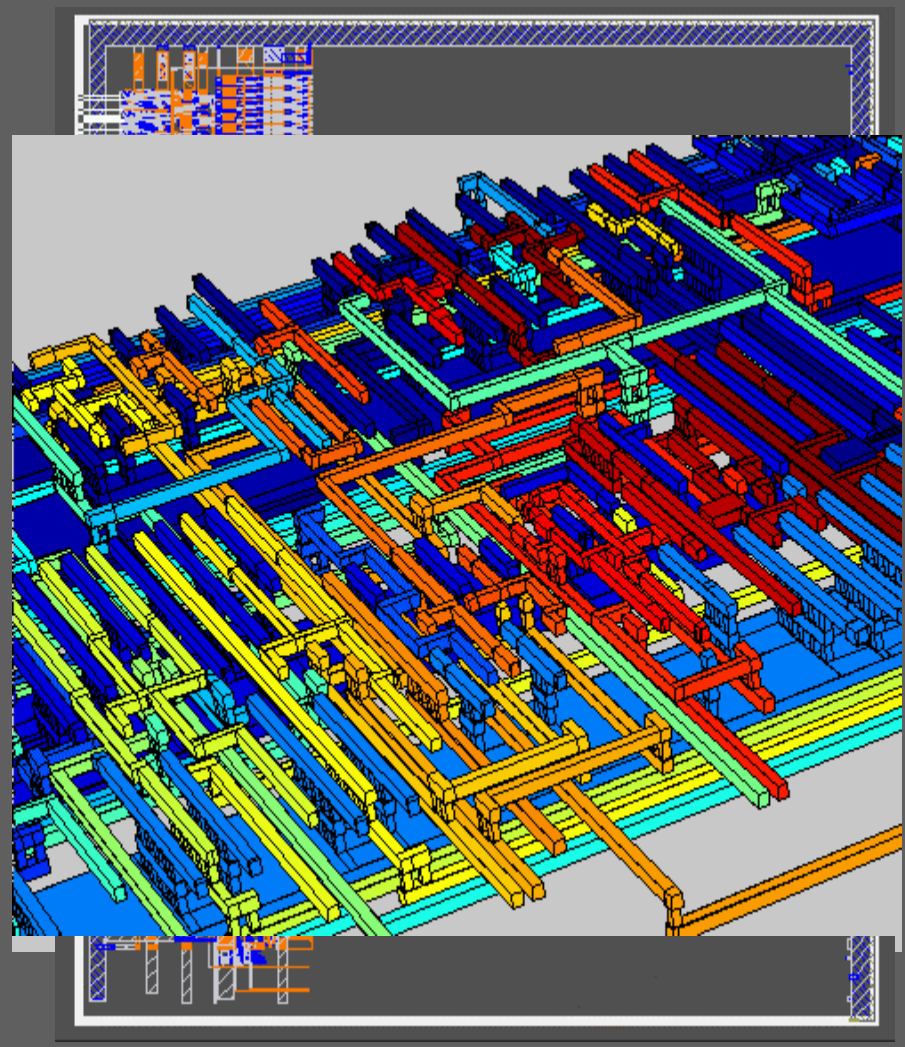
CORNING Intellisense Intellisuite™

MEMS Design

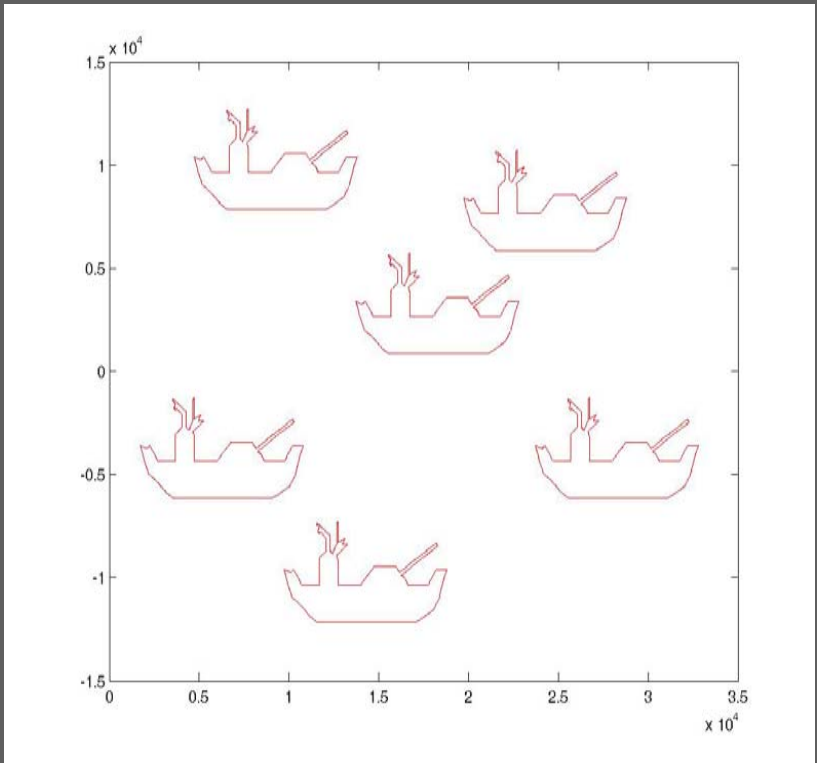
Gaussian98, Gaussian 03, Q-Chem

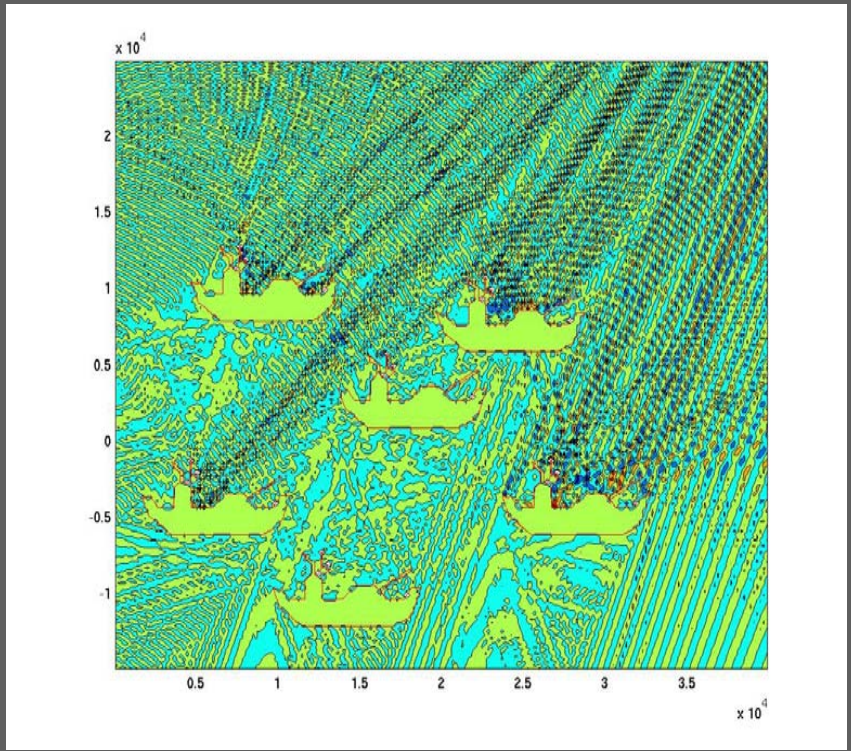
Nebula (Kapur/Long)

- Chip level capacitance calculation
- The scale of the geometric description is overwhelming
- *Billions* of geometric features



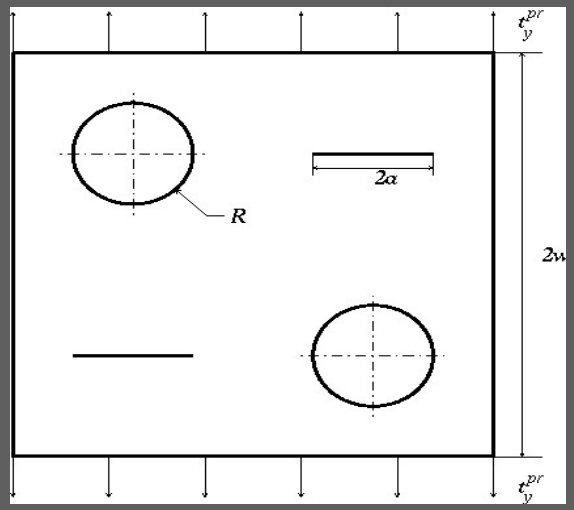
EM scattering: Wideband FMM

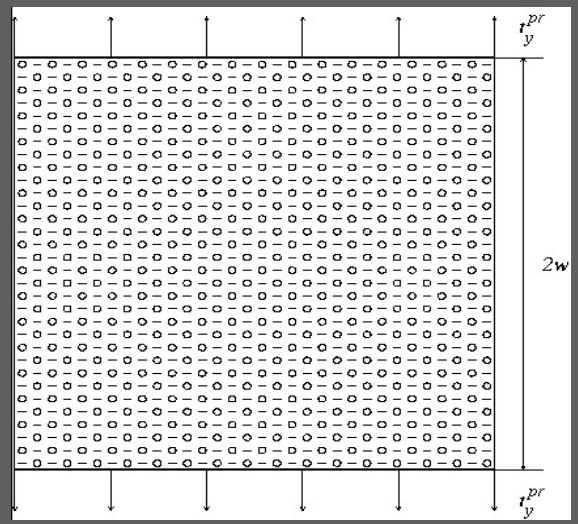




15,120 points, 10th order accuracy, 50λ / ship
5 minutes (1GHz Pentium 3 Laptop)

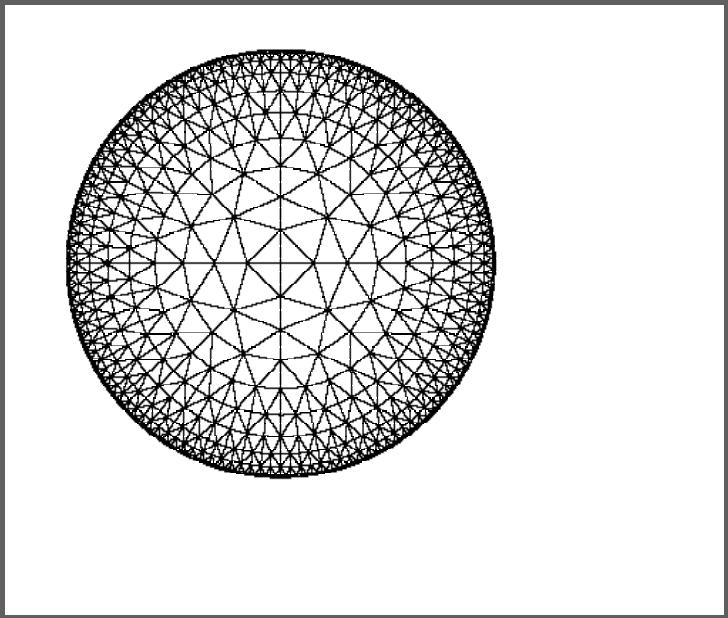
Linear Elasticity

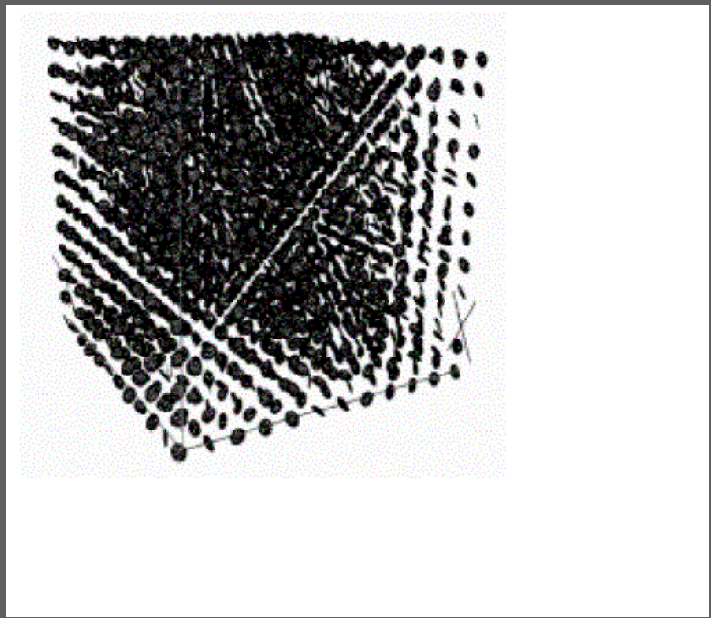




- Helsing and Jonsson (2002)
- 10,000 cracks – 500,000 boundary points
  10 digit accuracy – 4 hours SUN Ultra 10

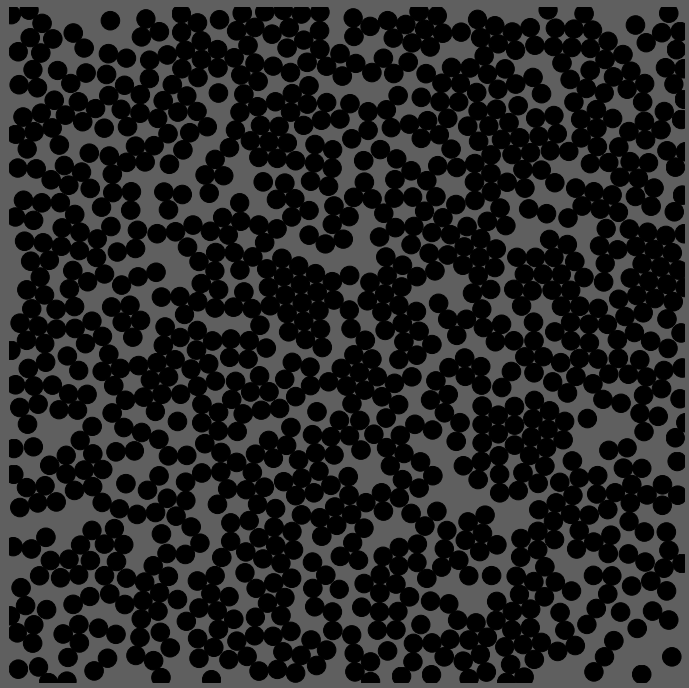
Linear Elasticity





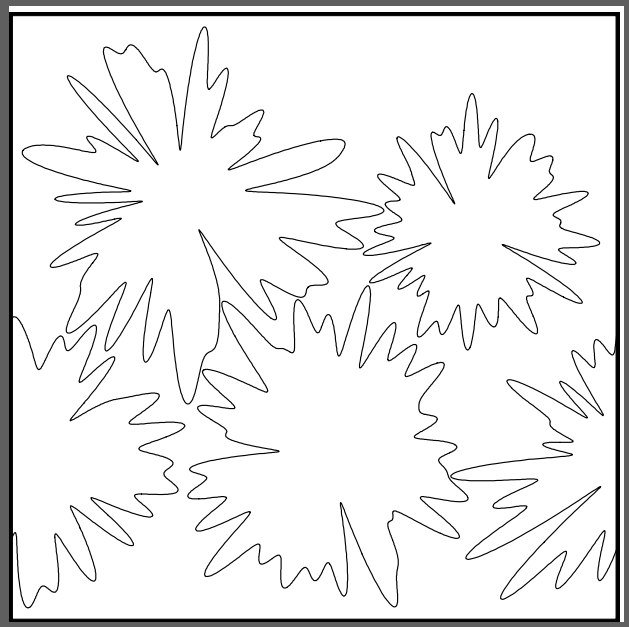
- Yoshida, Nishimura, Kobayashi (*J Structural Eng,* 2001)
- 12 x 12 x 12 penny shaped cracks
- 1.3M surface triangles, 2hrs., DEC alpha 500MHz

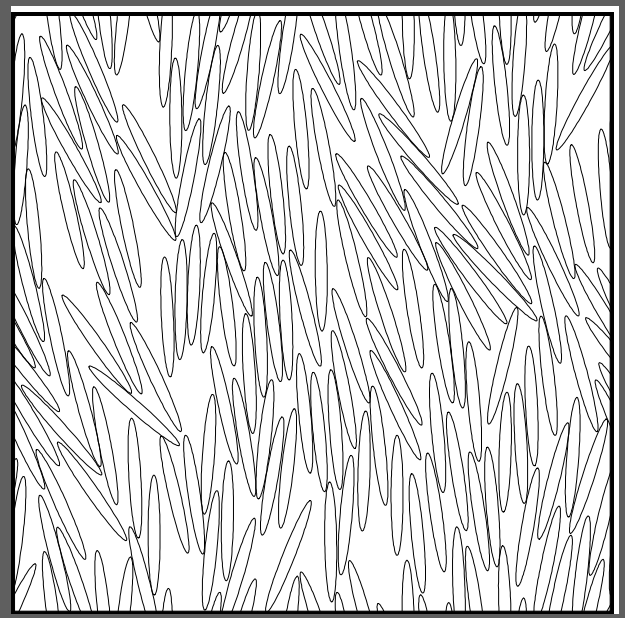
Random composites



– Cheng and G- (1997)

Complex Materials

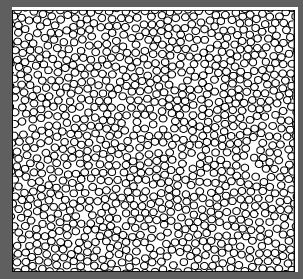


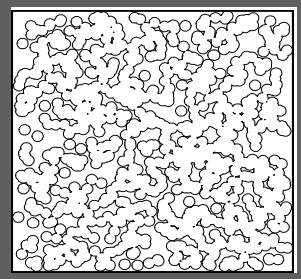


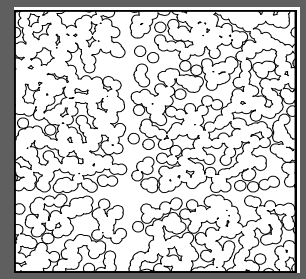
G- and Helsing (1996)

Complex Materials

Helsing (1997)



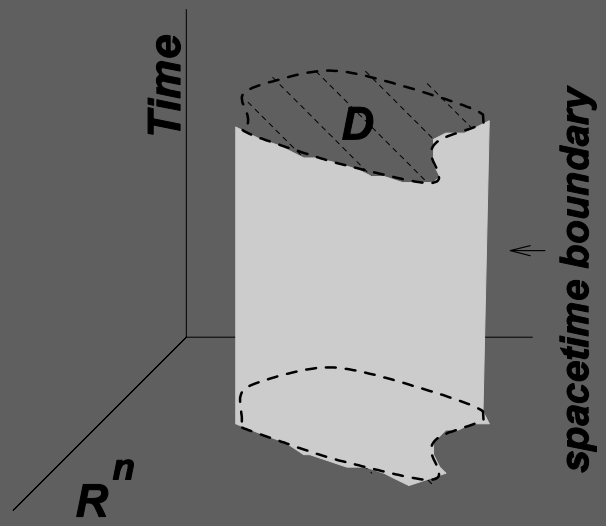




Time dependent Problems

- Diffusion, crystal growth
- Acoustics, Maxwell eqs

$$S(x) = \int_0^t \int_B G(x-y,t-s)\, h(y,s)\, dy\, ds$$ ⇒ N^2M^2 work



Some Fast Time-Domain Algorithms

- Heat equation: G-- & Strain (1991), G- & Lin (1998): O(NM) work
- Wave Equation: Ergin, Shanker, Aygun, Michielssen (1997,…): O(NM $\log^2 N$) work
- Nonreflecting Boundary Conditions :
  - Wave Equation: Alpert, G– Hagstrom (1998)
  - Schrodinger Equation: G- & Jiang (2002)

Summary

- Fast algorithms for potential problems are maturing as a technology. Directly applicable to dislocation dynamics and MD.
- Current research is extending this capability to variable coefficient PDEs in several dimensions.
- Can be used as preconditioners for more complex physics modeling
- Hierarchical numerical library design is critical for verification and supportability

- Materials design is both quantum mechanical and an inverse problem. Fast algorithms can play a supporting role in accelerating simulation methods, but breakthroughs are likely to come only from improved physical/phenomenological modeling