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Fast Algorithms and Parallel Computing:
Solution of Extremely Large Real-Life Problems in Computational Electromagnetics

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Adjunct Professor, Dept. of ECE, University of Illinois at Urbana-Champaign

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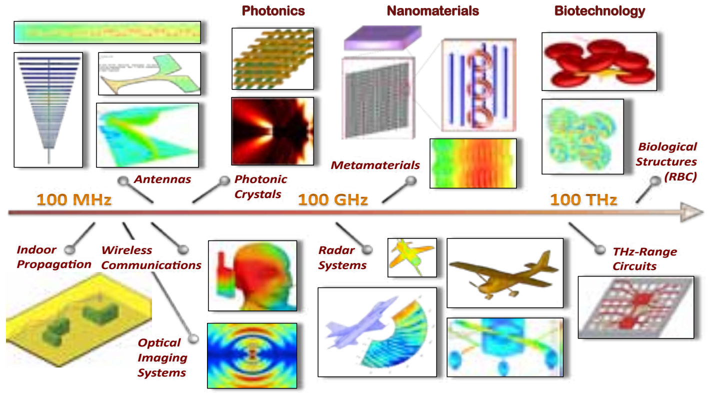
Real-Life Electromagnetics Problems
At Different Frequencies



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Radar Problem

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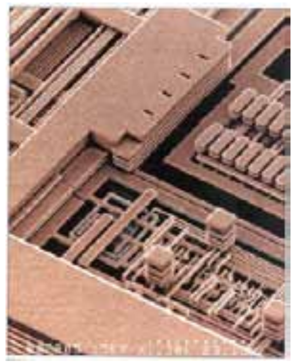
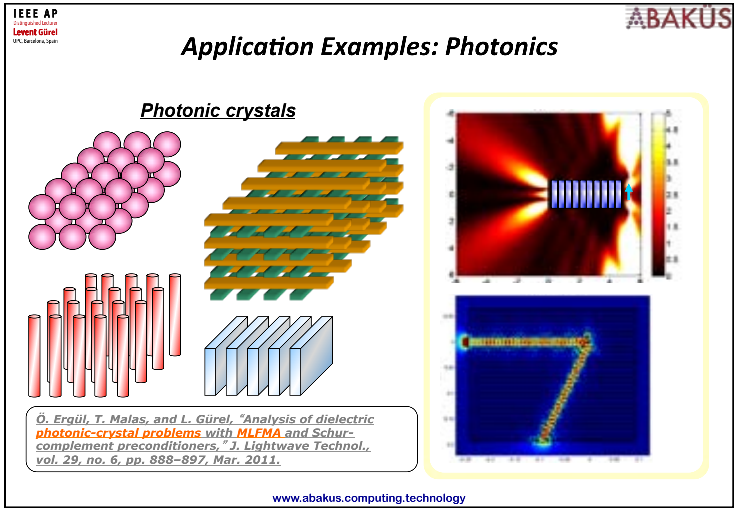
Real-Life Problem
Electromagnetic Modeling of Microcircuits

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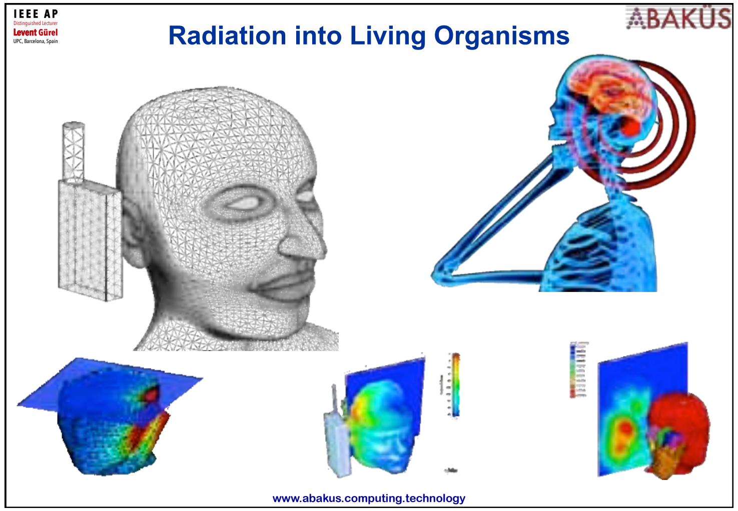
Application Examples: Photonics
Photonic crystals
Ö. Ergül, T. Malas, and L. Gürel, "Analysis of dielectric photonic-crystal problems with MLFMA and Schur-complement preconditioners," J. Lightwave Technol., vol. 29, no. 6, pp. 888–897, Mar. 2011.
www.abakus.computing.technology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Radiation into Living Organisms
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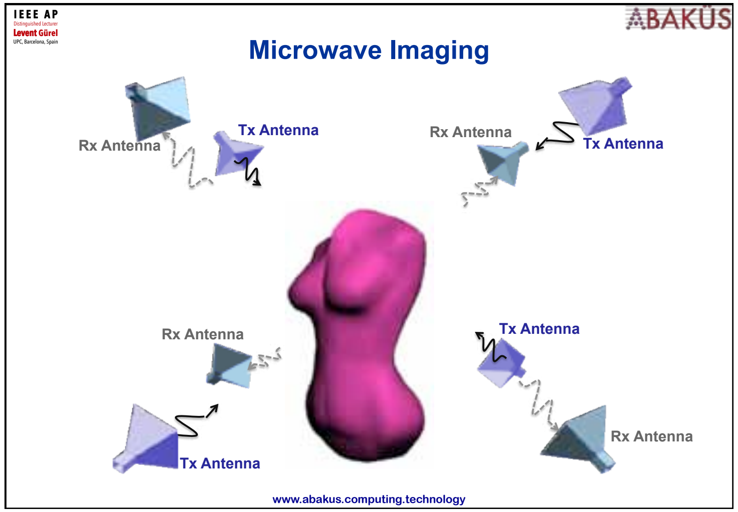
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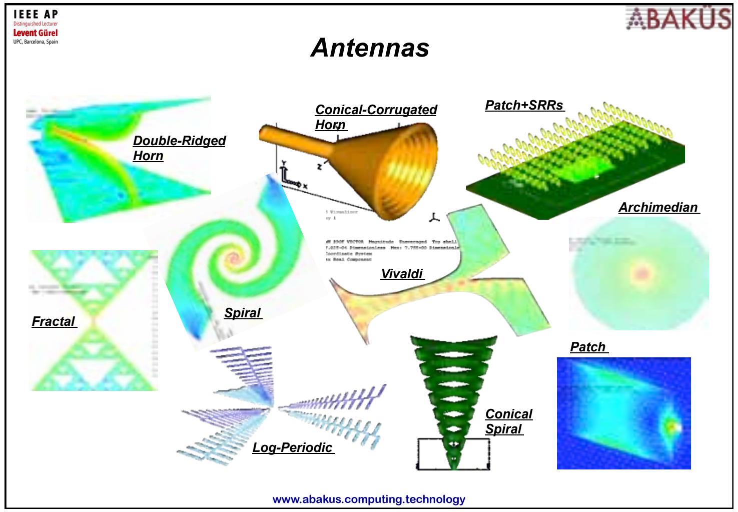
Microwave Imaging
Rx Antenna
Tx Antenna
Rx Antenna
Tx Antenna
Rx Antenna
Tx Antenna
Tx Antenna
Rx Antenna
www.abakus.computing.technology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Antennas
Double-Ridged Horn
Conical-Corrugated Horn
Patch+SRRs
Archimedian
Vivaldi
Fractal
Spiral
Log-Periodic
Conical Spiral
Patch
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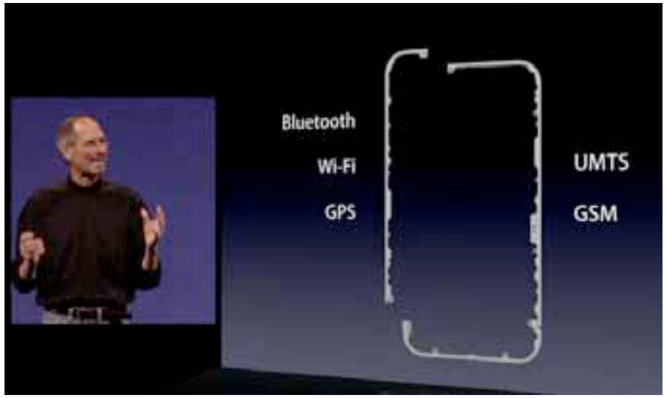
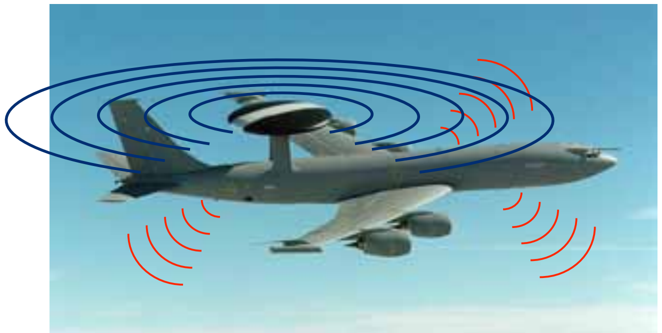
Mobile Device Antennas



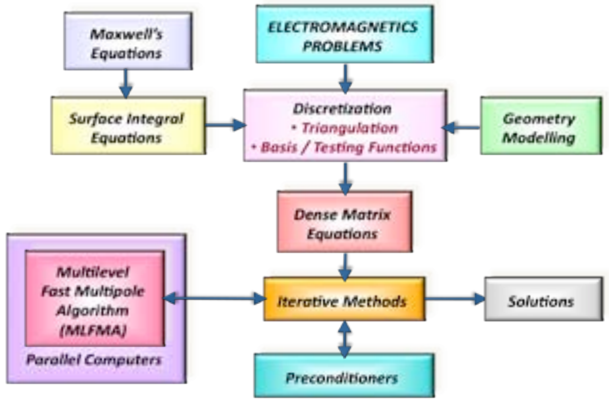
Satellite Antennas

Antennas Mounted on Platforms



- Interaction of multiple antennas
- Characteristics of mounted antennas (different from isolated antennas)
- Optimization of the placement of the antennas

Simulation Environment



Maxwell's Equations

$$\nabla \times \bar{E}(\bar{r},t) = -\frac{\partial}{\partial t}\bar{B}(\bar{r},t)$$

$$\nabla \times \bar{H}(\bar{r},t) = \frac{\partial}{\partial t}\bar{D}(\bar{r},t) + \bar{J}(\bar{r},t)$$

$$\nabla \cdot \bar{B}(\bar{r},t) = 0$$

$$\nabla \cdot \bar{D}(\bar{r},t) = \rho(\bar{r},t)$$

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Surface Integral Equations

- ***Electric-Field Integral Equation (EFIE):***

$$-\hat{\boldsymbol{t}}(\boldsymbol{r}) \cdot ik \int_{S'} d\boldsymbol{r}' \left(\bar{\boldsymbol{I}} - \frac{\nabla\nabla'}{k^2} \right) g(\boldsymbol{r},\boldsymbol{r}') \cdot \boldsymbol{J}(\boldsymbol{r}') = \frac{1}{\eta}\hat{\boldsymbol{t}}(\boldsymbol{r}) \cdot \boldsymbol{E}^{inc}(\boldsymbol{r})$$

- ***Magnetic-Field Integral Equation (MFIE):***

$$\boldsymbol{J}(\boldsymbol{r}) - \hat{\boldsymbol{n}}(\boldsymbol{r}) \times \int_{S'} d\boldsymbol{r}' \boldsymbol{J}(\boldsymbol{r}') \times \nabla' g(\boldsymbol{r},\boldsymbol{r}') = \hat{\boldsymbol{n}}(\boldsymbol{r}) \times \boldsymbol{H}^{inc}(\boldsymbol{r})$$

- ***Combined-Field Integral Equation (CFIE):***

$$\text{CFIE} = \alpha\text{EFIE} + (1-\alpha)\text{MFIE}$$

- ***Hybrid-Field Integral Equation (HFIE):***

$$\text{HFIE} = \alpha(\boldsymbol{r})\text{EFIE} + \left[1 - \alpha(\boldsymbol{r})\right]\text{MFIE}$$

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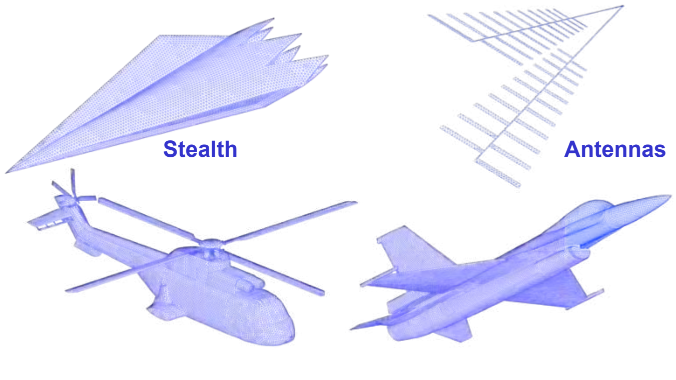
Geometry Discretization



Mesh Size: λ/10

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Discretization

$$\boldsymbol{J}(\boldsymbol{r}) = \sum_{n=1}^{N} a_n \boldsymbol{b}_n(\boldsymbol{r})$$

Number of unknowns

- **Matrix equations:**

$$\sum_{n=1}^{N} Z_{mn}^{E,M,C,H} a_n = v_m^{E,M,C,H}, \qquad m = 1,2,\ldots N$$

Basis functions

- **Matrix elements:**

$$Z_{mn}^{E} = \int_{S_m} d\boldsymbol{r}\; \boldsymbol{t}_m(\boldsymbol{r}) \cdot \int_{S_n} d\boldsymbol{r}'\; \bar{\boldsymbol{G}}(\boldsymbol{r},\boldsymbol{r}') \cdot \boldsymbol{b}_n(\boldsymbol{r}')$$

Testing functions

$$Z_{mn}^{M} = \int_{S_m} d\boldsymbol{r}\; \boldsymbol{t}_m(\boldsymbol{r}) \cdot \boldsymbol{b}_n(\boldsymbol{r}) - \int_{S_m} d\boldsymbol{r}\; \boldsymbol{t}_m(\boldsymbol{r}) \cdot \hat{\boldsymbol{n}} \times \int_{S_n} d\boldsymbol{r}'\; \boldsymbol{b}_n(\boldsymbol{r}') \times \nabla' g(\boldsymbol{r},\boldsymbol{r}')$$

$$Z_{mn}^{C} = \alpha Z_{mn}^{E} + (1-\alpha)\frac{i}{k} Z_{mn}^{M} \qquad Z_{mn}^{H} = \alpha_m Z_{mn}^{E} + (1-\alpha_m)\frac{i}{k} Z_{mn}^{M}$$

Matrix Elements…

…are electromagnetic interactions

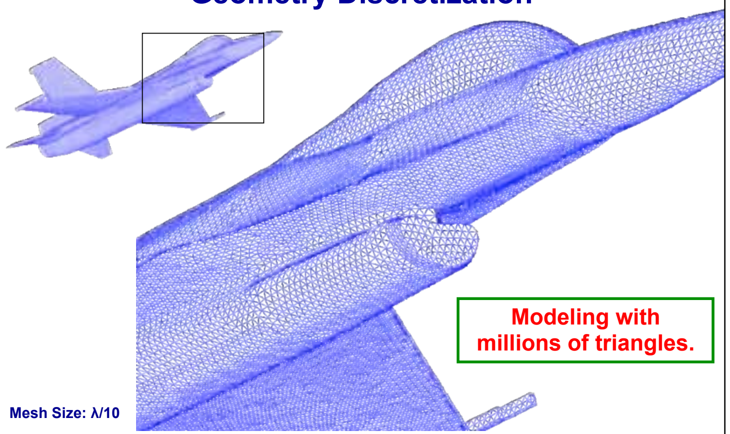
$$Z_{mn}^{E} = \int_{S_m} d\boldsymbol{r}\, \boldsymbol{t}_m(\boldsymbol{r}) \cdot \int_{S_n} d\boldsymbol{r}'\; \bar{G}(\boldsymbol{r},\boldsymbol{r}') \cdot \boldsymbol{b}_n(\boldsymbol{r}')$$

Testing functions

Basis functions

$$\sum_{n=1}^{N} Z_{mn}^{E} a_n = v_m^{E}, \quad m = 1,2,\ldots N$$

Geometry Discretization



Matrix Equation

System of Linear Equations

$$\boldsymbol{A} \cdot \boldsymbol{x} = \boldsymbol{b}$$

$$\boldsymbol{Z} \cdot \boldsymbol{a} = \boldsymbol{v}$$

Two Equations with Two Unknowns

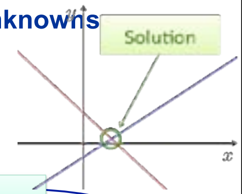
$$\begin{cases} x + y = 12 \\ 2x - 3y = 14 \end{cases}$$

Three Equations with Three Unknowns

$$\begin{cases} (a)\ 3x - 8y + z = -14 \\ (b)\ x - y + z = -5 \\ (c)\ x - 3y = -4 \end{cases}$$

Two Equations with Two Unknowns

$$\begin{cases} x + y = 12 \\ 2x - 3y = 14 \end{cases}$$



Cramer's Rule

$$x = \frac{\begin{vmatrix} 12 & 1 \\ 14 & -3 \end{vmatrix}}{\begin{vmatrix} 1 & 1 \\ 2 & -3 \end{vmatrix}} = \frac{12\cdot(-3) - 1\cdot 14}{1\cdot(-3) - 1\cdot 2} = \frac{-50}{-5} = 10$$

$$y = \frac{\begin{vmatrix} 1 & 12 \\ 2 & 14 \end{vmatrix}}{\begin{vmatrix} 1 & 1 \\ 2 & -3 \end{vmatrix}} = \frac{1\cdot(14) - 12\cdot 4}{1\cdot(-3) - 1\cdot 2} = \frac{-10}{-5} = 2$$

$x = 12 - y$
$y = 2$
$x = 12 - 2$
$x = 10$

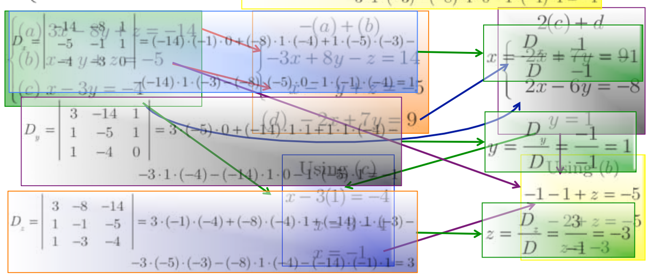
Three Equations with Three Unknowns

$$\begin{cases} 3x - 8y + z = -14 \\ x - y + z = -5 \\ x - 3y = -4 \end{cases}$$

Cramer's Rule

Two Equations with Two Unknowns

$$D = \begin{vmatrix} 3 & -8 & 1 \\ 1 & -1 & 1 \\ 1 & -3 & 0 \end{vmatrix} = 3\cdot(-1)\cdot 0 + (-8)\cdot 1\cdot 1 + 1\cdot 1\cdot(-3) - 3\cdot 1\cdot(-3) - (-8)\cdot 1\cdot 0 - 1\cdot(-1)\cdot 1 = -1$$



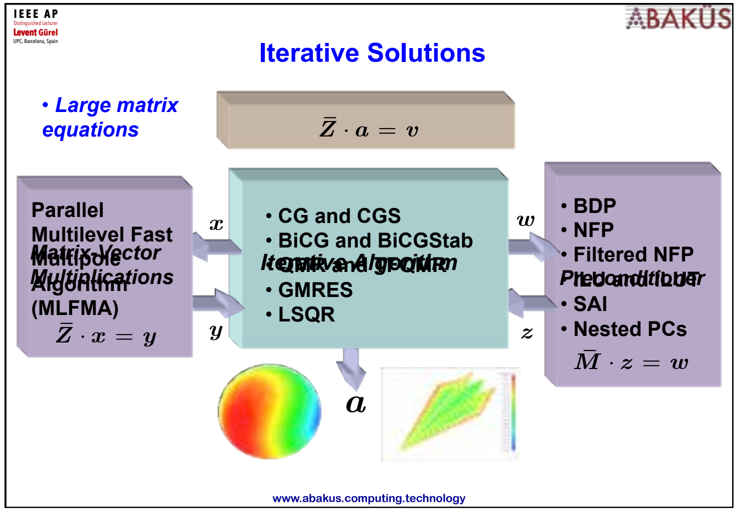
Matrix Equation

System of Linear Equations

$$Z \cdot a = v$$

Algorithmic Complexity

- Gaussian Elimination: $O(N^3)$
- Cramer Rule: $O(N!)$, $O(N^3)$
- Iterative Methods: $O(kN^2)$
- Fast Algorithms: $O(N \log N)$, $O(N)$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Iterative Solutions
• Large matrix equations
$\bar{Z} \cdot a = v$
Parallel Multilevel Fast Multipole Algorithm (MLFMA)
Matrix-Vector Multiplications
$\bar{Z} \cdot x = y$
x
y
• CG and CGS
• BiCG and BiCGStab
• QMR and tfQMR
• GMRES
• LSQR
Iterative Algorithm
w
z
• BDP
• NFP
• Filtered NFP
• ILU and ILUT
• SAI
• Nested PCs
Preconditioner
$\bar{M} \cdot z = w$
a
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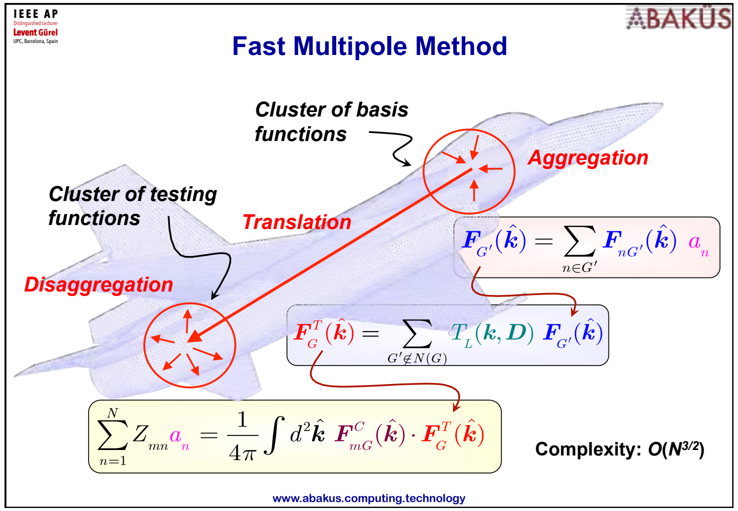
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Fast Multipole Method
Cluster of basis functions
Aggregation
Cluster of testing functions
Translation
Disaggregation
$F_{G'}(\hat{k}) = \sum_{n \in G'} F_{nG'}(\hat{k})\, a_n$
$F^T_G(\hat{k}) = \sum_{G' \notin N(G)} T_L(k, D)\, F_{G'}(\hat{k})$
$\sum_{n=1}^{N} Z_{mn} a_n = \frac{1}{4\pi} \int d^2\hat{k}\, F^C_{mG}(\hat{k}) \cdot F^T_G(\hat{k})$
Complexity: $O(N^{3/2})$
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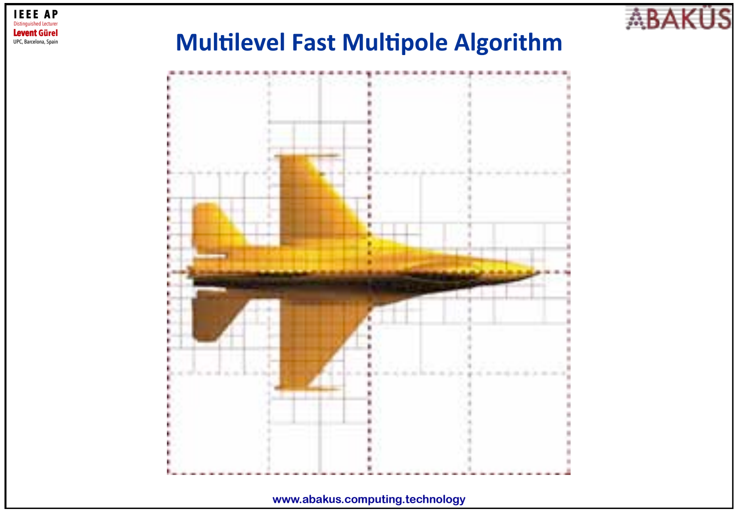
IEEE AP
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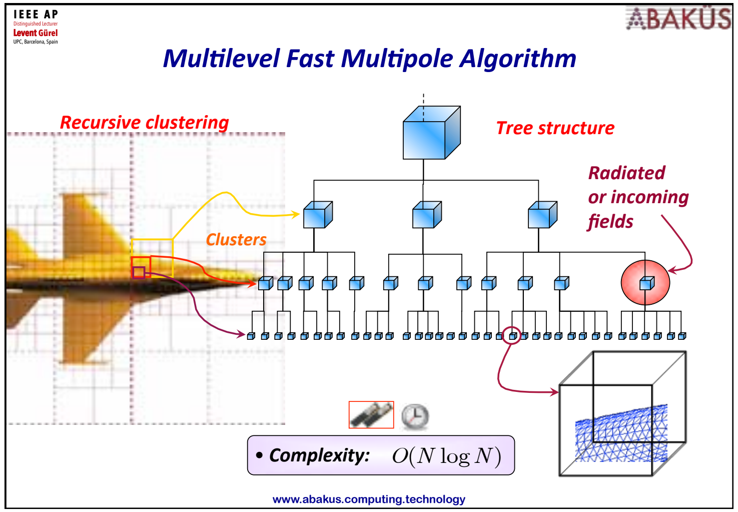
ABAKÜS
Multilevel Fast Multipole Algorithm
www.abakus.computing.technology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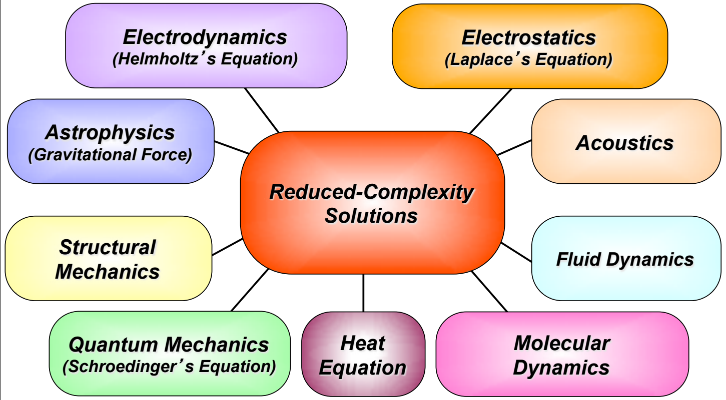
ABAKÜS
Multilevel Fast Multipole Algorithm
Recursive clustering
Tree structure
Radiated or incoming fields
Clusters
• Complexity: $O(N \log N)$
www.abakus.computing.technology

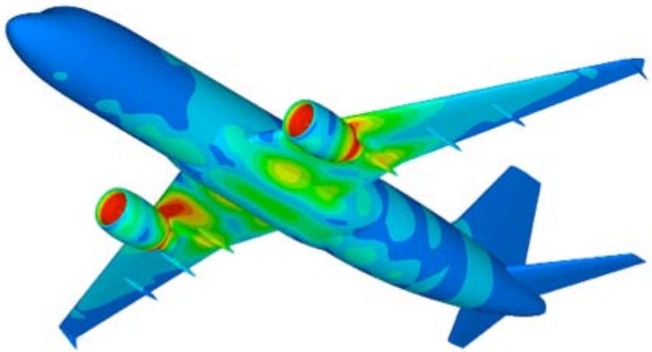
Fast Multipole Methods



Acoustics and Elastics

- Y. H. Chen, W. C. Chew, and S. Zeroug, "Fast multipole method as an efficient solver for 2D elastic wave surface integral equations," Computational Mechanics, vol. 20, pp. 495-506, 1997.
- M. S. Tong, W. C. Chew, and M. J. White, "Multilevel fast multipole algorithm for acoustic wave scattering by truncated ground with trenches," Journal of Acoustic Society of America, vol. 123, no. 5, pp. 2513-2521, 2008.
- M. S. Tong and W. C. Chew, "Multilevel fast multipole algorithm for elastic wave scattering by large 3D objects," Journal of Computational Physics, vol. 228, no. 3, pp. 921-932, 2009.

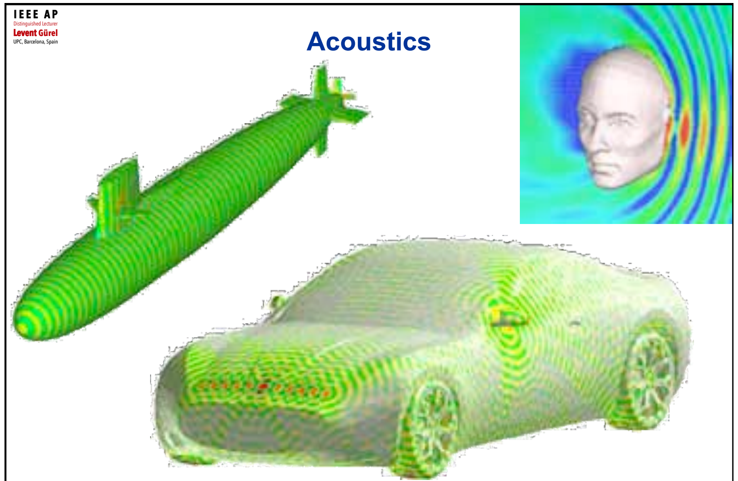
Acoustics



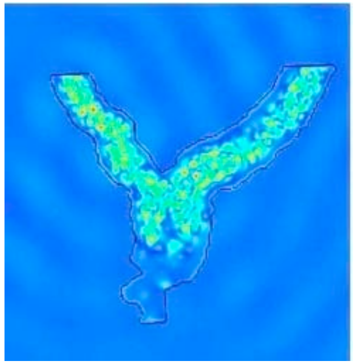
Noise Control

This is an exterior acoustic wave radiation problem. Total complex DOFs = 541,152, solved on a desktop PC

Acoustics



Seismic Wave Propagation



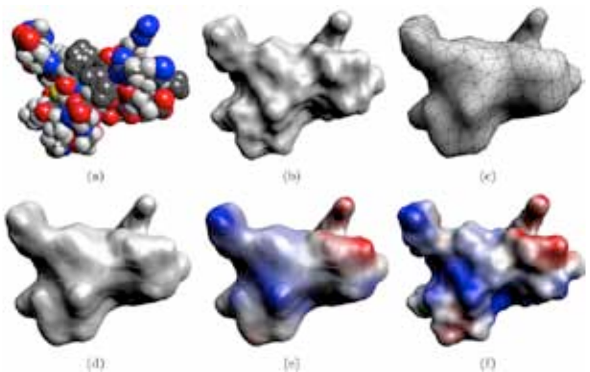
S. Chaillat, J.F. Semblat, M. Bonnet, A preconditioned 3-D multi-region fast multipole solver for seismic wave propagation in complex geometries. Communications in Computational Physics (special issue WAVES 2009), Vol. 11, 594-609, 2012.

Schrödinger's Equation

- **Volumetric fast multipole method for modeling Schrödinger's equation**

Zhiqin Zhao, Narayan Kovvali, Wenbin Lin, Chang-Hoi Ahn, Luise Couchman, Lawrence Carin
Department of Electrical and Computer Engineering, Duke University, Durham, NC 27708-0291, USA; Naval Research Laboratory, Washington, DC, USA; School of Electronic Engineering, University of Electronic Science and Technology of China, Chengdu, China, Journal of Computational Physics (Impact Factor: 2.14). 06/2007; DOI: 10.1016/j.jcp.2006.11.003

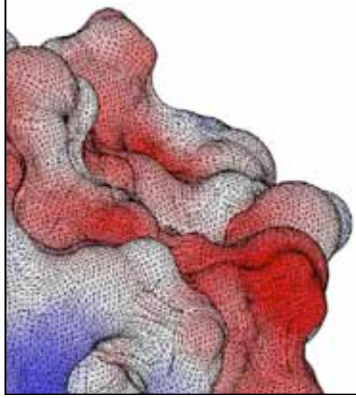
Molecular Electrostatics

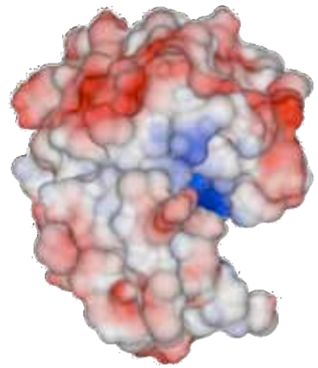


AN EFFICIENT HIGHER-ORDER FAST MULTIPOLE BOUNDARY ELEMENT SOLUTION FOR POISSON-BOLTZMANN BASED MOLECULAR ELECTROSTATICS
Chandrajit Bajaj, Shun-Chuan Chen, and Alexander Rand
SIAM J Sci Comput. Jan 1, 2011; 33(2): 826–848.

Molecular model of a protein (PDB id:1PPE, 436 atoms). (a) The van der Waals surface of the protein which models the molecule as a union of balls. (b) The variational molecular surface gives a smooth approximation of the van der Waals surface. (c) The variational surface is then triangulated and then decimated to produce a smaller mesh. This decimated mesh contains 1,000 triangles. (d) The algebraic spline molecular surface (ASMS) fits a smooth surface over the triangular mesh. (e) Electrostatic potential computed using the 1,000 patch ASMS. (f) Electrostatic potential using an ASMS with 74,812 patches. The surfaces in (e) and (f) are colored by the electrostatic potential, ranging from −3.8 kbT/ec (red) to +3.8 kbT/ec (blue).

Biomolecular Electrostatics





Surface charge plot on a lysozyme molecule
Validation of the PyGBe code for Poisson-Boltzmann equation with boundary element methods
Christopher D. Cooper, Lorena A. Barba
George Washington University

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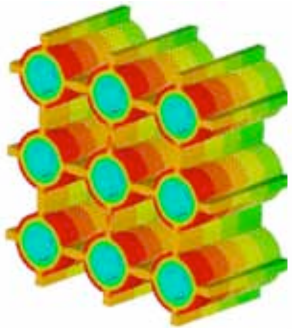
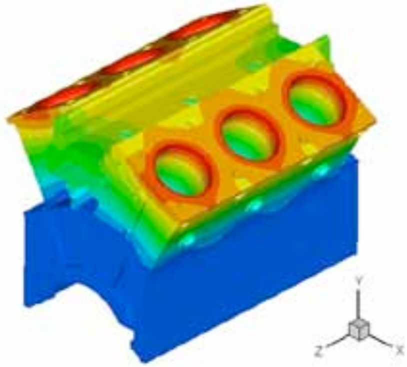
Thermal Analysis



Fuel Cells
There are 9,000 small side holes in this model!
Total DOFs = 530,000, solved on a desktop PC)
Dr. Yijun Liu, CAE Research Lab, University of Cincinnati
http://urbana.mie.uc.edu/yliu/Software/



Engine Block

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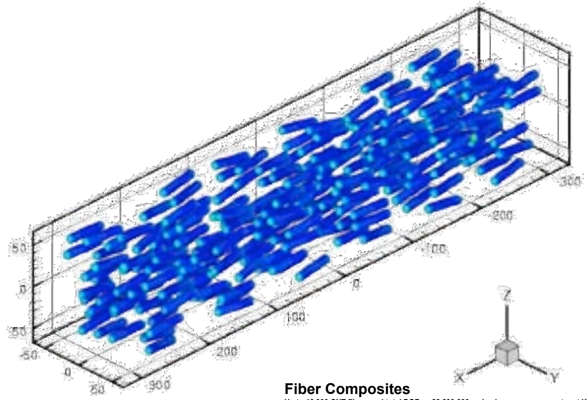
Elasticity



Fiber Composites
Up to 16,000 CNT fibers and total DOFs = 28,800,000, solved on a supercomputer at Kyoto University
http://urbana.mie.uc.edu/yliu/Images/FMM_BEM.JPG

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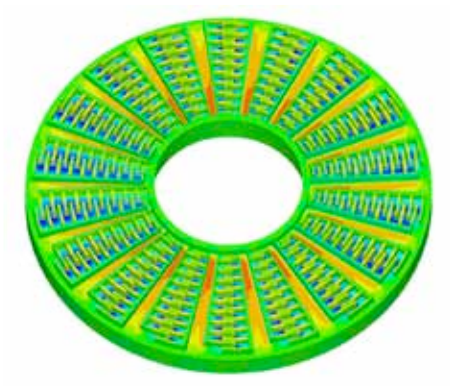
Stokes Flow



MEMS
This is an exterior Stokes flow problem. Total DOFs = 1,087,986, solved on a desktop PC

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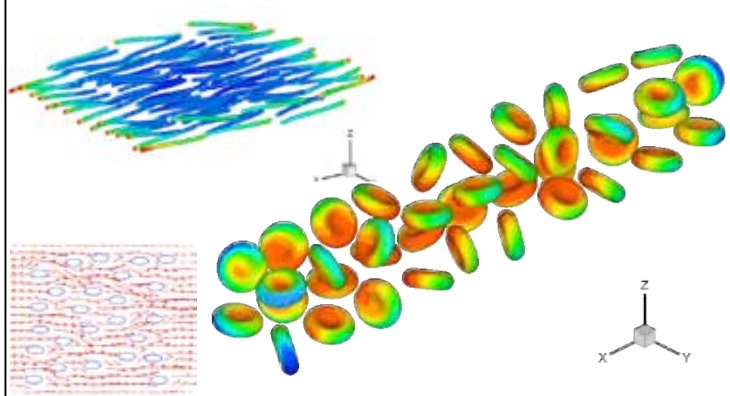
Stokes Flow



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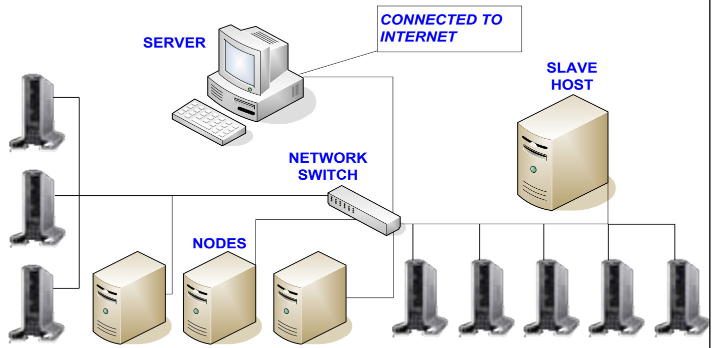
Books

Parallel Computing

Constructing a Parallel Computer Cluster



Parallel Computers

Parallel Computing

Constructing Parallel Computer Clusters

Not in www.top500.org!!!

64-Core Cluster

8 nodes
Per node: Two Intel Xeon 5345 Quad-Core Processors
Total of 64 cores
Per node: 32 GB DDR2-667 533 MHz RAM
Total of 256 GB of RAM
Network: Infiniband

136-Core Cluster

Per node: Two Intel Xeon 5472 3 GHz Quad-Core Processors
Total of 136 cores
Per node: GB DDR2-667 533 MHz RAM
Total of 544 GB of RAM
Network: Infiniband

What is the Main Source of Efficiency?

N Unknowns	$O(N^3)$ Gaussian Elimination	$O(N^2)$ Iterative MOM (MVM)	$O(N^{3/2})$ Single-Level FMM	$O(N \log N)$ Multi-Level FMM
1000	1 s	2 s	4 s	8 s
10^6	32 years	23 days	35 h	7 h
10^7	32 K years	6.3 years	46 days	89 h
10^8	32 M years	630 years	4 years	46 days
10^9	32 G years	63 K years	127 years	1.5 years (555 days)

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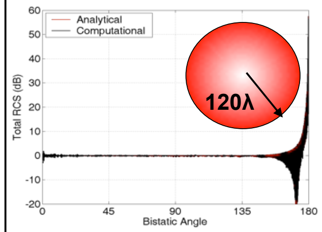
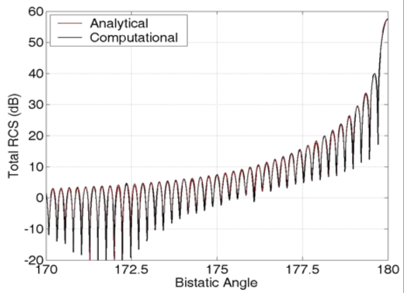
53 Million Unknowns

Sphere with radius of 120λ and diameter of 240λ

November 2007

53,112,384 Unknowns





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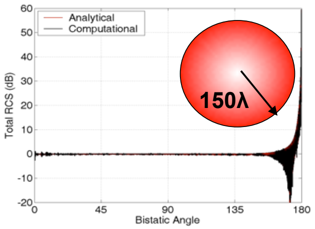
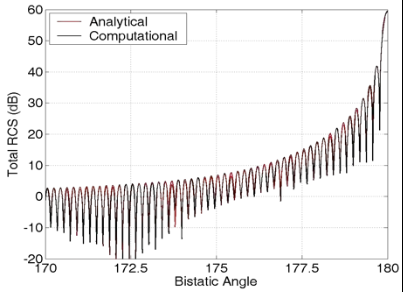
69 Million Unknowns

Sphere with radius of 150λ and diameter of 300λ

December 2007

69,177,600 Unknowns





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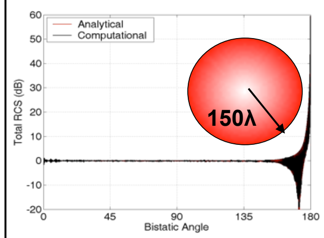
85 Million Unknowns

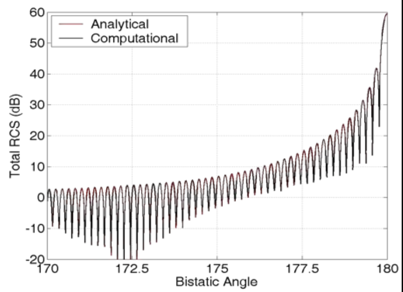
January 2008

Sphere with radius of 150λ and diameter of 300λ

Scattering results are compared to analytical values to demonstrate the accuracy of the numerical solution.

85,148,160 Unknowns





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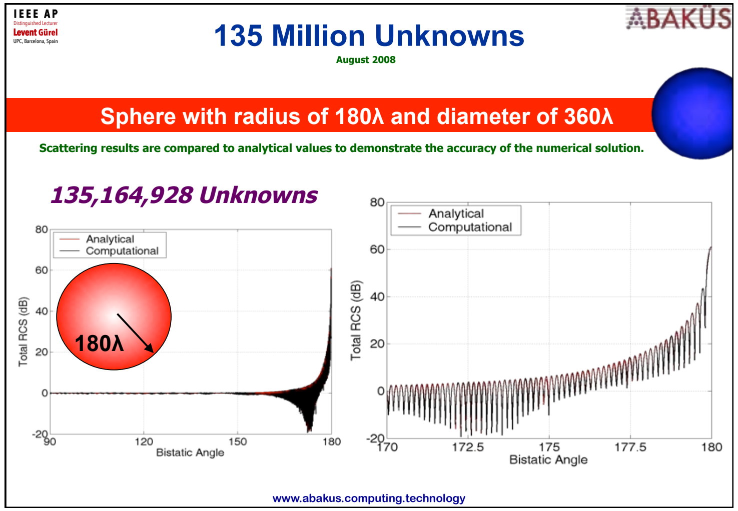
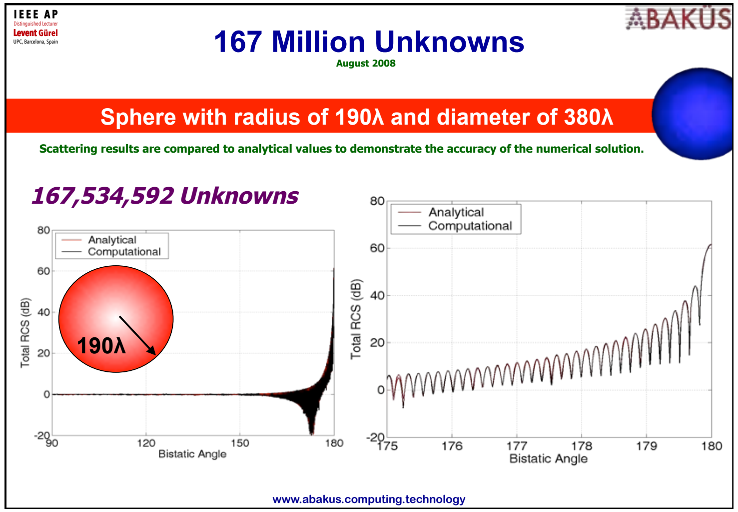
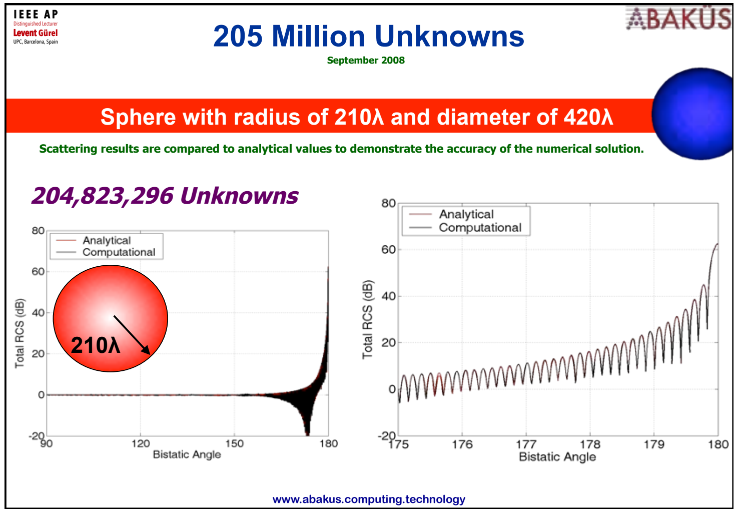
IEEE AP
Levent Gürel
ABAKÜS
Intel Pamphlet on the World Record
intel
Leap ahead
Case Study
Breakthrough in Scientific Computing:
BiLCEM Sets World Record in
Computational Electromagnetics
BiLCEM
Available at
www.cem.bilkent.edu.tr
www.abakus.computing.technology


IEEE AP
Levent Gürel
ABAKÜS
135 Million Unknowns
August 2008
Sphere with radius of 180λ and diameter of 360λ
Scattering results are compared to analytical values to demonstrate the accuracy of the numerical solution.
135,164,928 Unknowns
180λ
Analytical
Computational
Total RCS (dB)
Bistatic Angle
www.abakus.computing.technology


IEEE AP
Levent Gürel
ABAKÜS
167 Million Unknowns
August 2008
Sphere with radius of 190λ and diameter of 380λ
Scattering results are compared to analytical values to demonstrate the accuracy of the numerical solution.
167,534,592 Unknowns
190λ
Analytical
Computational
Total RCS (dB)
Bistatic Angle
www.abakus.computing.technology


IEEE AP
Levent Gürel
ABAKÜS
205 Million Unknowns
September 2008
Sphere with radius of 210λ and diameter of 420λ
Scattering results are compared to analytical values to demonstrate the accuracy of the numerical solution.
204,823,296 Unknowns
210λ
Analytical
Computational
Total RCS (dB)
Bistatic Angle
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IEEE AP
Levent Gürel

ABAKÜS

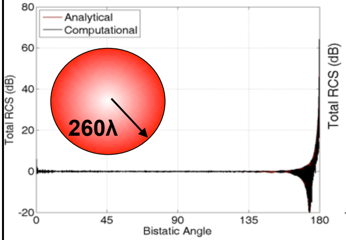
307 Million Unknowns

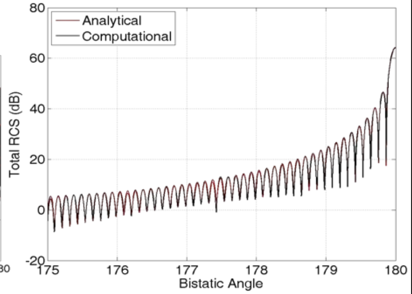
December 2009

Sphere with radius of 260λ and diameter of 520λ

Scattering results are compared to analytical values to demonstrate the accuracy of the numerical solution.

307,531,008 Unknowns





IEEE AP
Levent Gürel

ABAKÜS

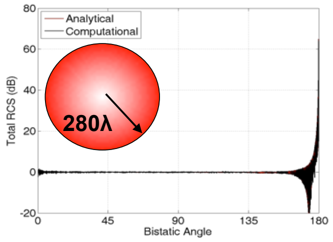
375 Million Unknowns

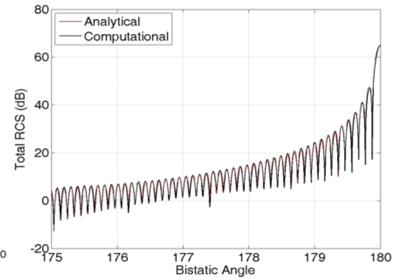
December 2009

Sphere with radius of 280λ and diameter of 560λ

Scattering results are compared to analytical values to demonstrate the accuracy of the numerical solution.

374,490,624 Unknowns





IEEE AP
Levent Gürel

ABAKÜS

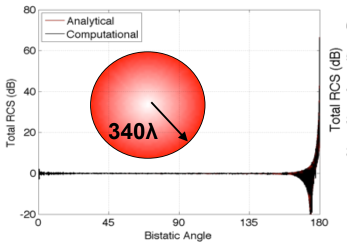
540 Million Unknowns

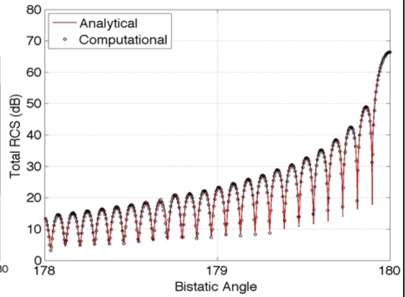
September 2010

Sphere with radius of 340λ and diameter of 680λ

Scattering results are compared to analytical values to demonstrate the accuracy of the numerical solution.

540,659,712 Unknowns



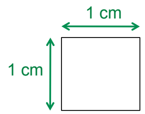


IEEE AP
Levent Gürel

ABAKÜS

How Large are Large Matrix Equations?

Each element of the matrix is a complex number with real and imaginary parts



7.654321E+02
+ j 1.234567E-03

If we could fit each element of the matrix in a square of 1 cm by 1 cm…

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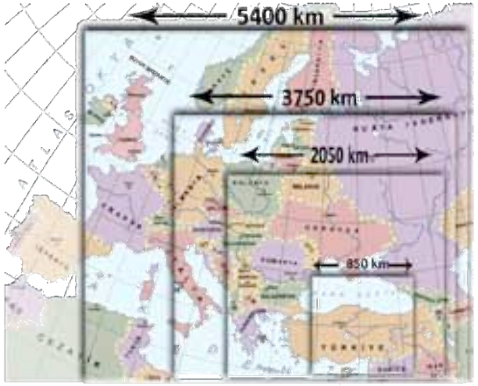
ABAKÜS

How Large are Large Matrix Equations?



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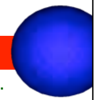
670 Million Unknowns

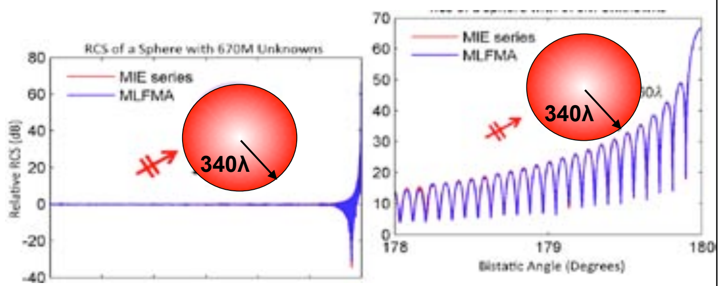
2013



Sphere with radius of 340λ and diameter of 680λ

Scattering results are compared to analytical values to demonstrate the accuracy of the numerical solution.

670 Million Unknowns



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IEEE AP
Levent Gürel

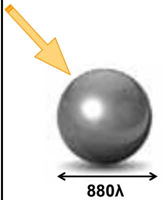
ABAKÜS

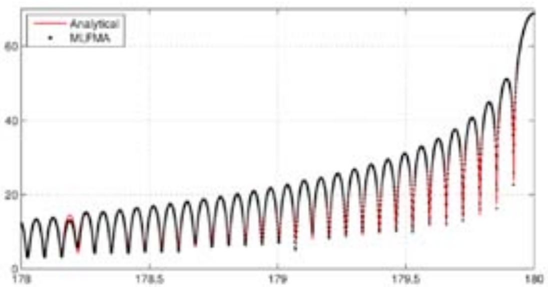
850 Million Unknowns

2014

Sphere with radius of 440λ and diameter of 880λ

Scattering results are compared to analytical values to demonstrate the accuracy of the numerical solution.





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IEEE AP
Levent Gürel

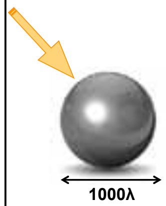
ABAKÜS

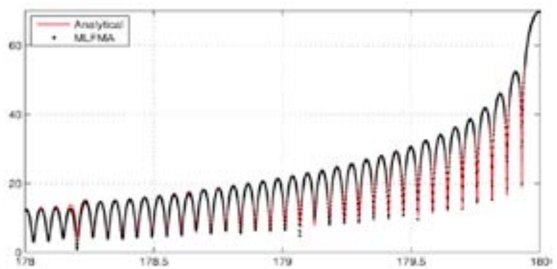
1.1 Billion Unknowns

2014

Sphere with radius of 500λ and diameter of 1000λ

Scattering results are compared to analytical values to demonstrate the accuracy of the numerical solution.





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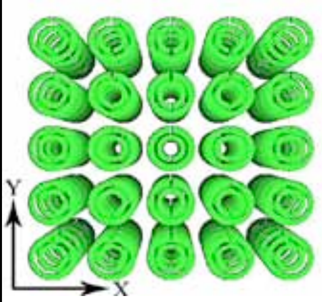
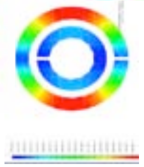
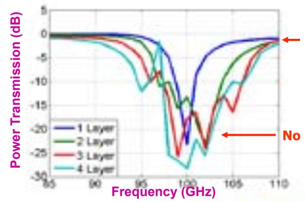
Nanomaterials: Metamaterials

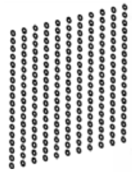
Split-Ring Resonators

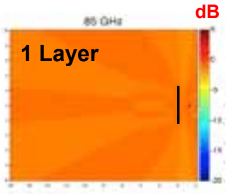


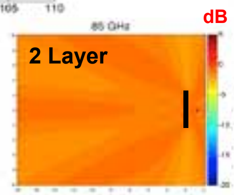


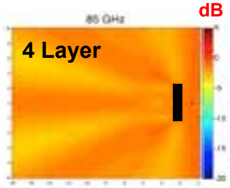
SRR Walls







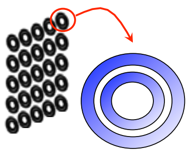




Meta Property: Stop band in frequency!

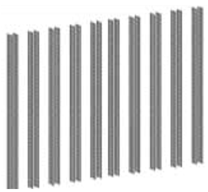
Special Configurations

Closed-Ring Resonators (CRRs)



All pass!

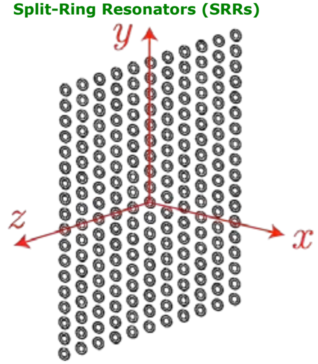
Thin Wire Array (TWA)



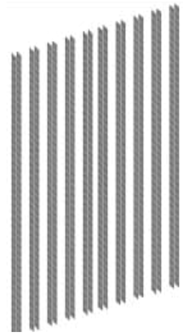
No pass!

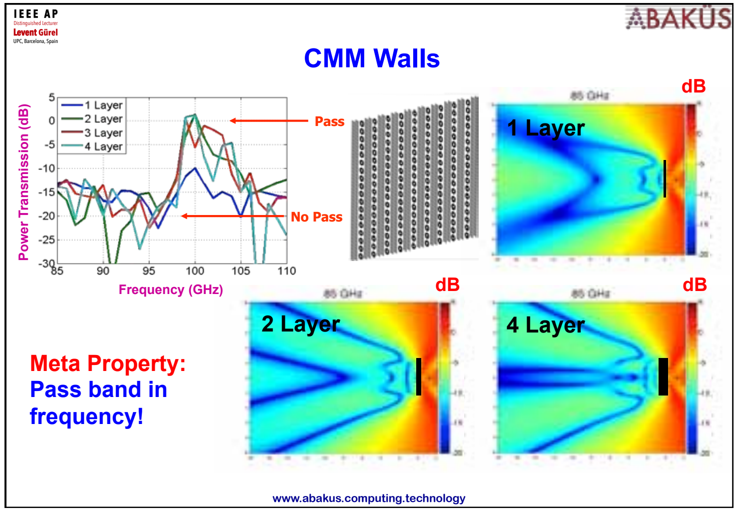
Composite Metamaterial (CMM)

Split-Ring Resonators (SRRs)



Thin Wire Array (TWA)




IEEE AP
Levent Gürel
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CMM Walls
Power Transmission (dB)
Frequency (GHz)
1 Layer
2 Layer
3 Layer
4 Layer
Pass
No Pass
dB
1 Layer
2 Layer
4 Layer
Meta Property:
Pass band in
frequency!
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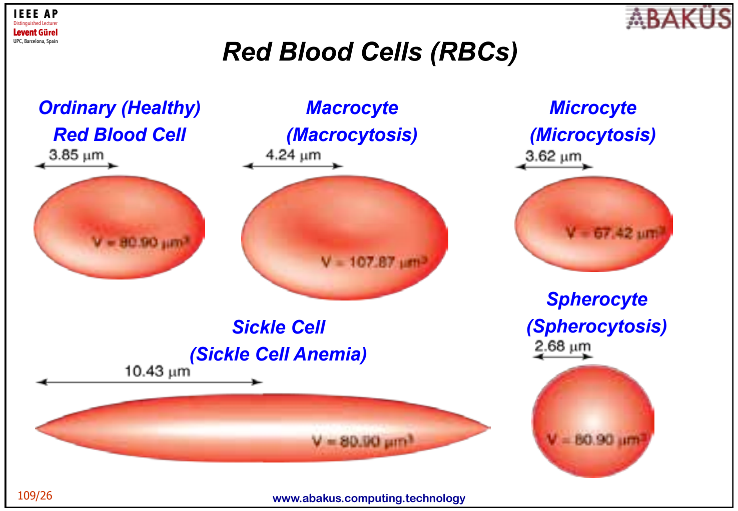
IEEE AP
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ABAKÜS
Red Blood Cells (RBCs)
Ordinary (Healthy)
Red Blood Cell
3.85 μm
V = 80.90 μm³
Macrocyte
(Macrocytosis)
4.24 μm
V = 107.87 μm³
Microcyte
(Microcytosis)
3.62 μm
V = 67.42 μm³
Sickle Cell
(Sickle Cell Anemia)
10.43 μm
V = 80.90 μm³
Spherocyte
(Spherocytosis)
2.68 μm
V = 80.90 μm³
109/26
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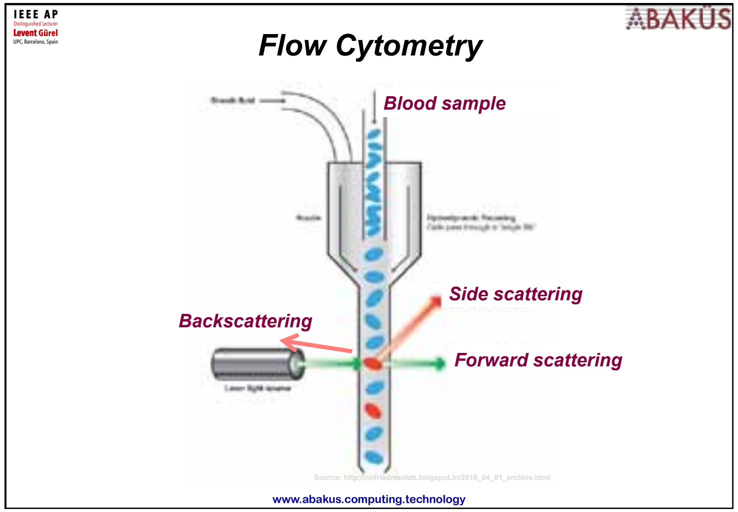
IEEE AP
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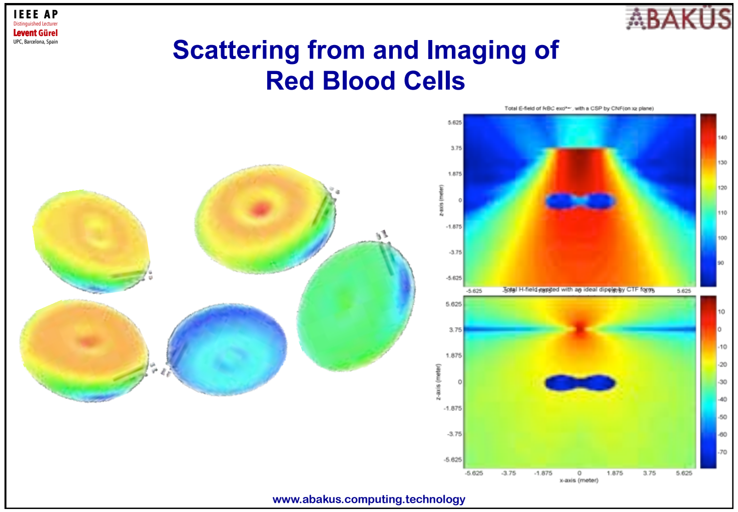
ABAKÜS
Flow Cytometry
Blood sample
Side scattering
Backscattering
Forward scattering
www.abakus.computing.technology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ABAKÜS
Scattering from and Imaging of
Red Blood Cells
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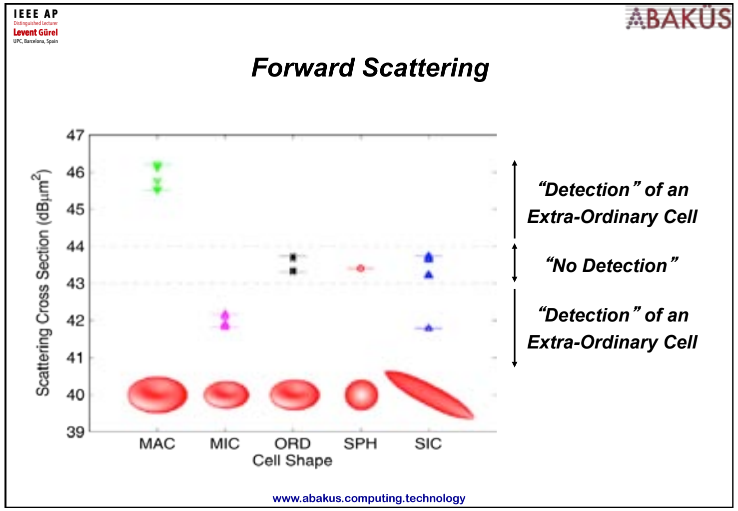
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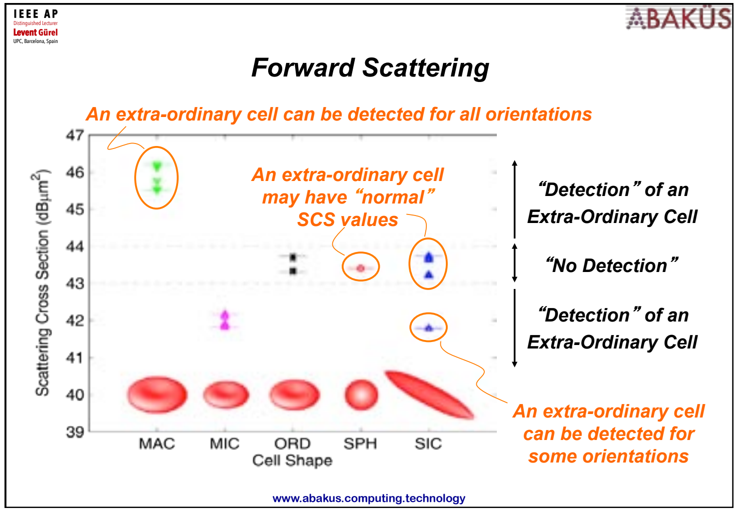
ABAKÜS
Forward Scattering
47
46
45
44
43
42
41
40
39
Scattering Cross Section (dBµm²)
MAC
MIC
ORD
SPH
SIC
Cell Shape
"Detection" of an Extra-Ordinary Cell
"No Detection"
"Detection" of an Extra-Ordinary Cell
www.abakus.computing.technology


IEEE AP
Levent Gürel
ABAKÜS
Forward Scattering
An extra-ordinary cell can be detected for all orientations
An extra-ordinary cell may have "normal" SCS values
47
46
45
44
43
42
41
40
39
Scattering Cross Section (dBµm²)
MAC
MIC
ORD
SPH
SIC
Cell Shape
"Detection" of an Extra-Ordinary Cell
"No Detection"
"Detection" of an Extra-Ordinary Cell
An extra-ordinary cell can be detected for some orientations
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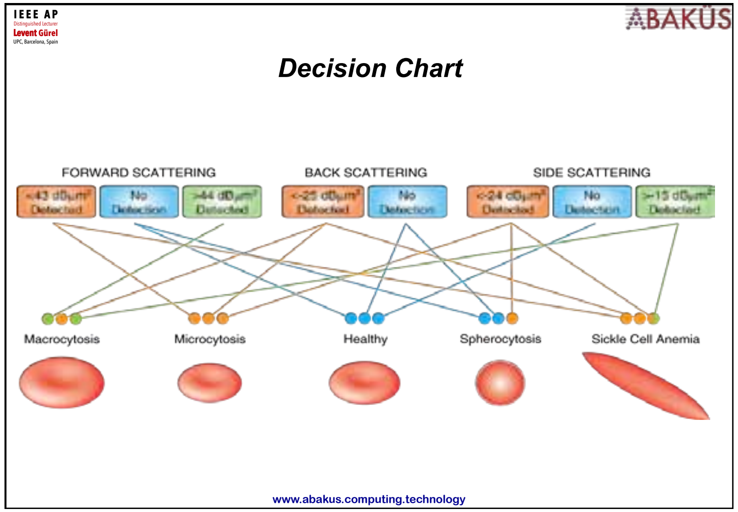
IEEE AP
Levent Gürel
ABAKÜS
Decision Chart
FORWARD SCATTERING
BACK SCATTERING
SIDE SCATTERING
No Detection
No Detection
No Detection
Macrocytosis
Microcytosis
Healthy
Spherocytosis
Sickle Cell Anemia
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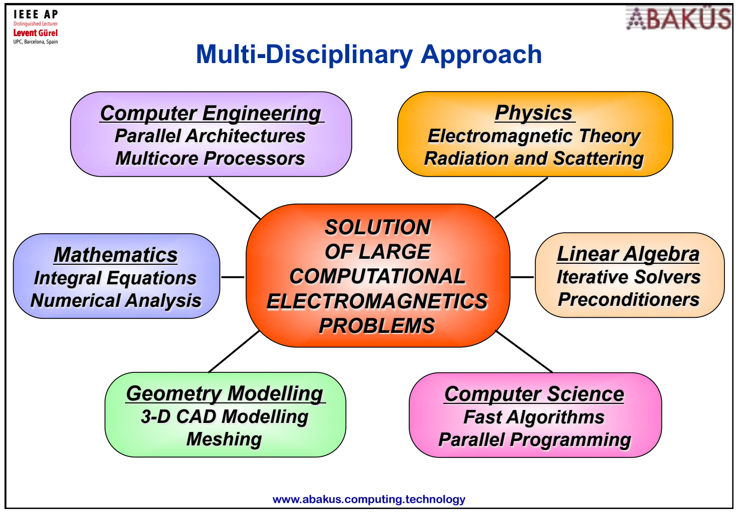
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Multi-Disciplinary Approach
Computer Engineering
Parallel Architectures
Multicore Processors
Physics
Electromagnetic Theory
Radiation and Scattering
Mathematics
Integral Equations
Numerical Analysis
SOLUTION OF LARGE COMPUTATIONAL ELECTROMAGNETICS PROBLEMS
Linear Algebra
Iterative Solvers
Preconditioners
Geometry Modelling
3-D CAD Modelling
Meshing
Computer Science
Fast Algorithms
Parallel Programming
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