Novel and Effective Preconditioners for Iterative Solvers

Fast Algorithms and Parallel Computing for the Solution of Extremely Large Integral Equations in Computational Electromagnetics

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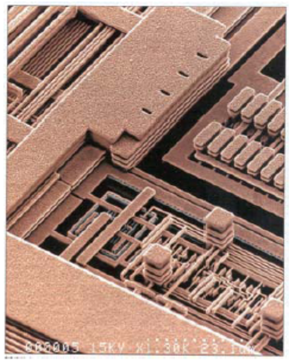
Prerequisites

- Maxwell's equations, Helmholtz equation
- Integral equations, surface integral equations
- Iterative solvers
- Fast multipole method(s) (FMM)
- Multi-level fast multipole algorithm (MLFMA)
- Parallel MLFMA
- Hierarchical Parallelization

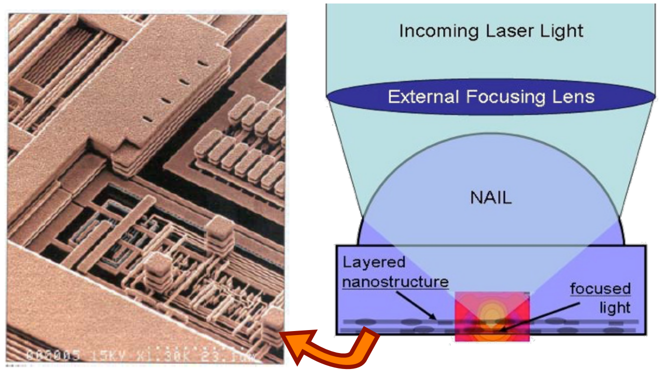
Real-Life Problem

Electromagnetic Modeling of Microcircuits



Real-Life Problem

Nano-Optical Imaging Systems



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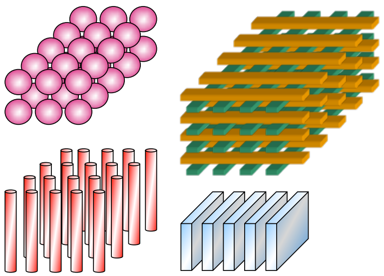
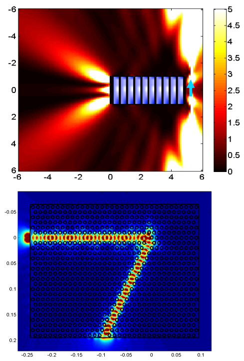
Examples to Dielectric Problems

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.

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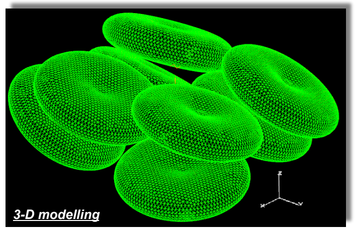
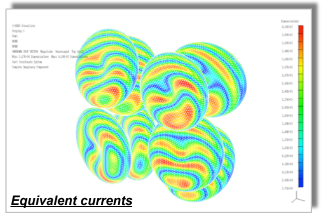
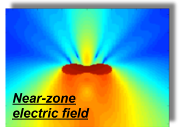
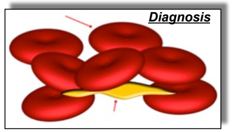
Examples to Dielectric Problems

Red blood cells









Ö. Ergül, A. Arslan-Ergül, and L. Gürel, "Computational study of scattering from healthy and diseased red blood cells using surface integral equations and the multilevel fast multipole algorithm," J. Biomed. Opt., vol. 15, no. 4, 045004, Jul./Aug. 2010.

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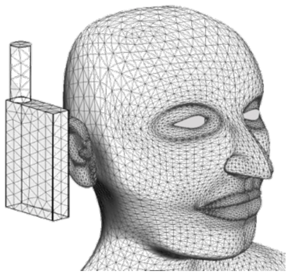
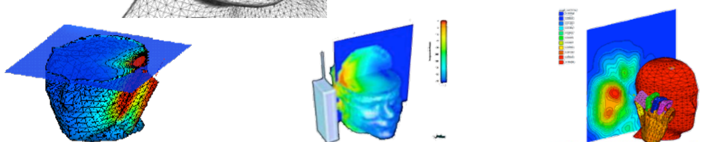
Radiation into Living Organisms





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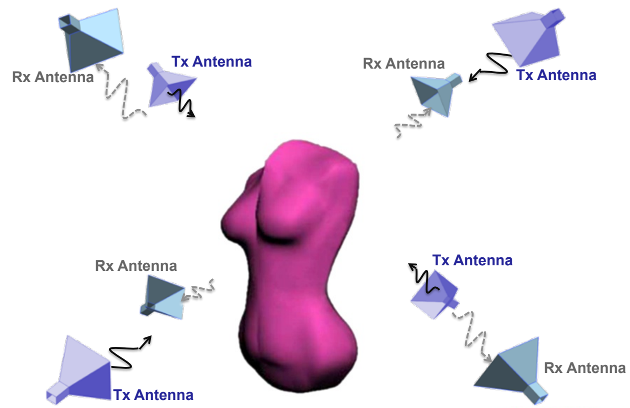
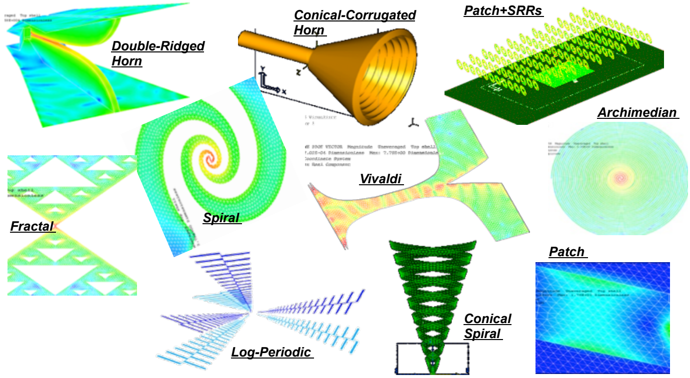
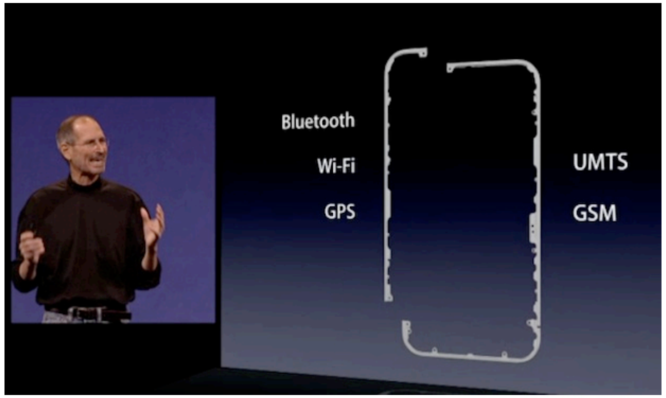
Microwave Imaging



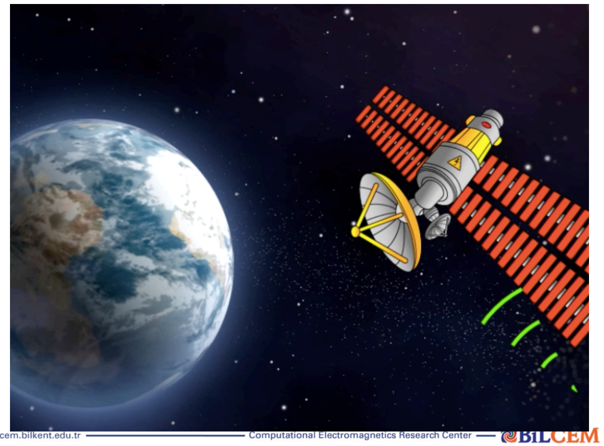
Antennas



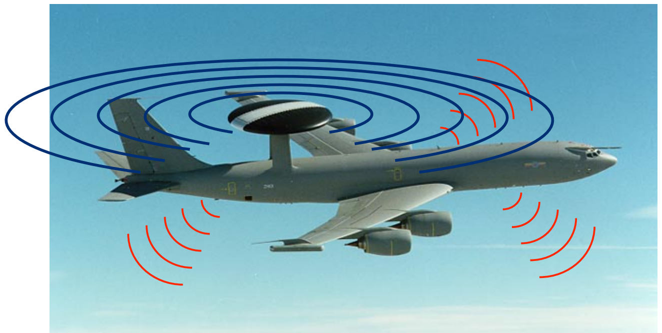
Mobile Device Antennas



Satellite Antennas

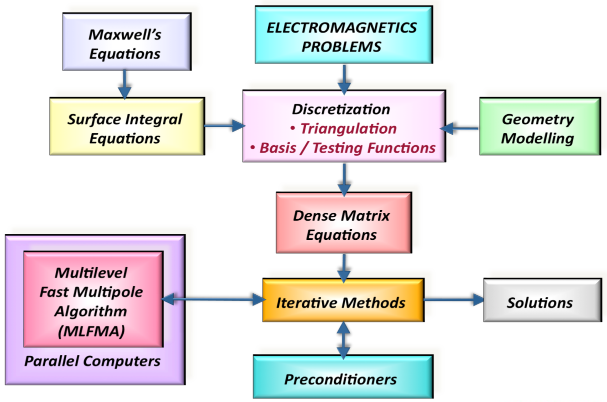


Antennas Mounted on Platforms



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

Simulation Environment



Maxwell's Equations

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

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

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

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

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):***

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

Discretization

Number of unknowns

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

- **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:**

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

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

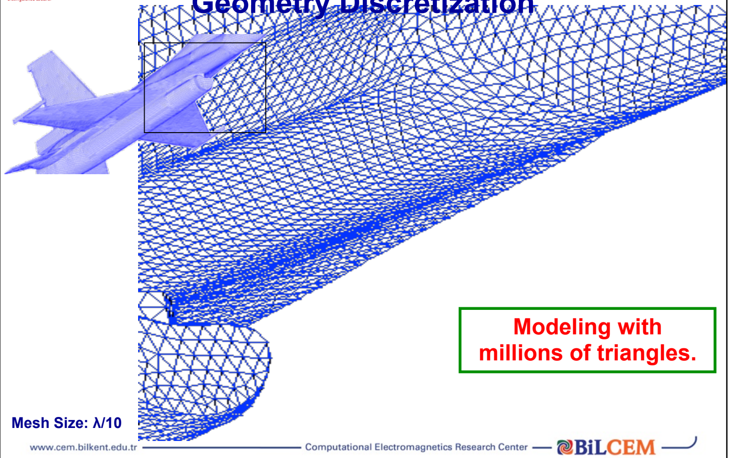
$$Z_{mn}^{E} = \int_{S_m} d\boldsymbol{r}\, \boldsymbol{t}_m(\boldsymbol{r}) \cdot \int_{S_n} d\boldsymbol{r}'\, \bar{G}(\boldsymbol{r},\boldsymbol{r}') \cdot \boldsymbol{b}_n(\boldsymbol{r}')$$

Testing functions

Basis functions

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

Geometry Discretization



Modeling with millions of triangles.

Mesh Size: λ/10

Matrix Equation

System of Linear Equations

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

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

Iterative Solutions

- *Large matrix equations*

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

Parallel Multilevel Fast Multipole Algorithm (MLFMA)

Matrix-Vector Multiplications

$\bar{Z} \cdot \boldsymbol{x} = \boldsymbol{y}$

$\boldsymbol{x}$, $\boldsymbol{y}$

Iterative Algorithm

- CG and CGS
- BiCG and BiCGStab
- QMR and TFQMR
- GMRES
- LSQR

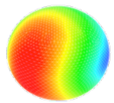
$\boldsymbol{w}$, $\boldsymbol{z}$

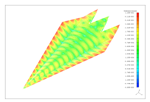
Preconditioner

- BDP
- NFP
- Filtered NFP
- ILU and ILUT
- SAI
- Nested PCs

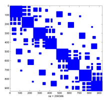
$\bar{M} \cdot \boldsymbol{z} = \boldsymbol{w}$

$\boldsymbol{a}$



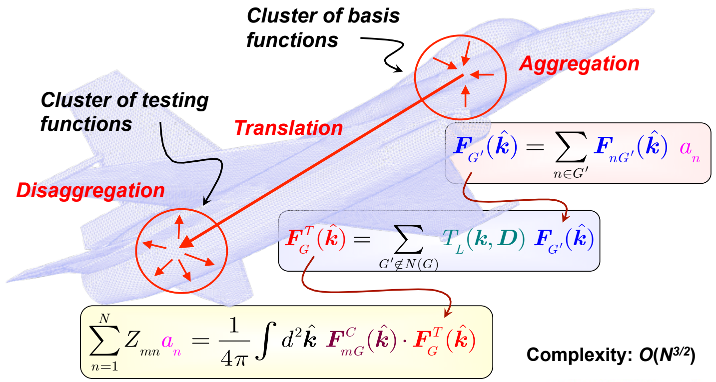


Preconditioners (for MLFMA)



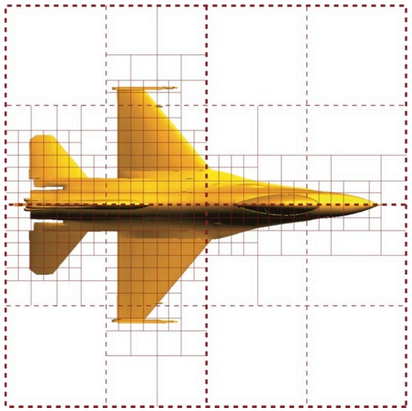
- ***Near-Field Preconditioners***
  - **LU** (too expensive)
  - **ILU: Incomplete LU**
  - **SAI: Sparse Approximate Inverse**
  - **INF: Iterative Near-Field Preconditioner**
- ***Full-Matrix Preconditioners (Approximate)***
  - **Use more than the available near-field matrix**
- ***Schur Preconditioners for Dielectric Formulations***

Fast Multipole Method

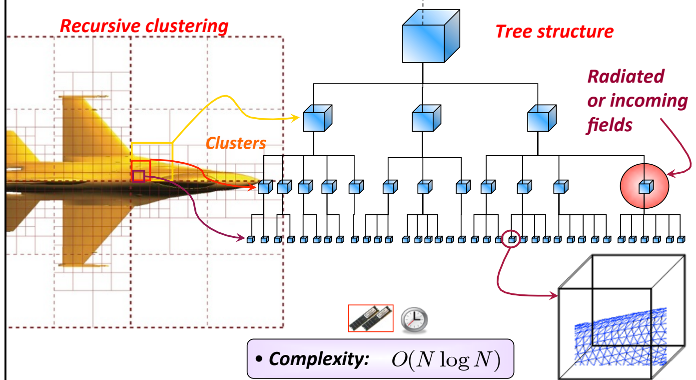


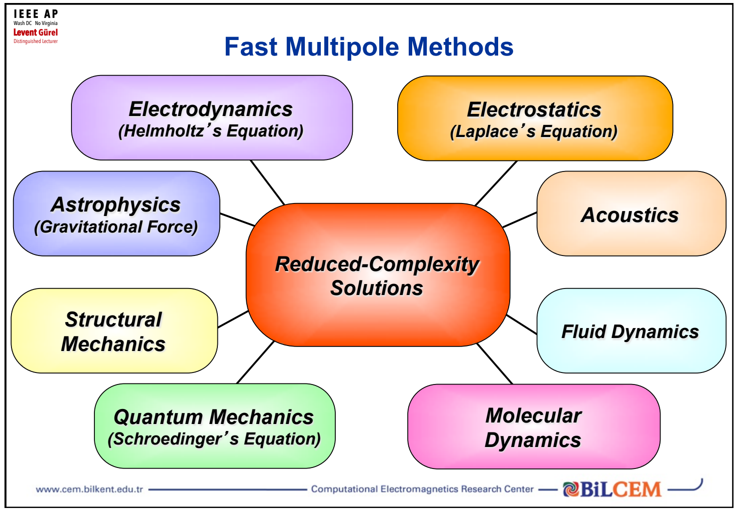
Complexity: $O(N^{3/2})$

Multilevel Fast Multipole Algorithm



Multilevel Fast Multipole Algorithm

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Fast Multipole Methods
Electrodynamics
(Helmholtz's Equation)
Electrostatics
(Laplace's Equation)
Astrophysics
(Gravitational Force)
Acoustics
Reduced-Complexity Solutions
Structural Mechanics
Fluid Dynamics
Quantum Mechanics
(Schroedinger's Equation)
Molecular Dynamics
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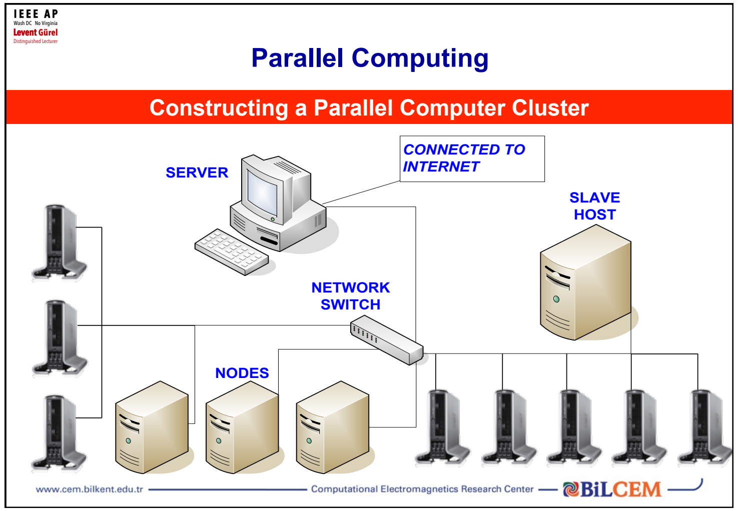
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Parallel Computing
Constructing a Parallel Computer Cluster
SERVER
CONNECTED TO INTERNET
SLAVE HOST
NETWORK SWITCH
NODES
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Parallel Computers
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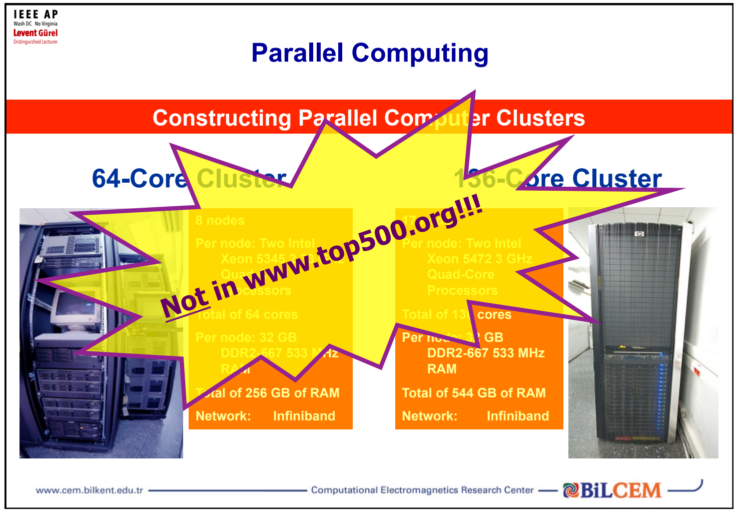
IEEE AP
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Parallel Computing
Constructing Parallel Computer Clusters
64-Core Cluster
8 nodes
Per node: Two Intel
Total of 64 cores
Per node: 32 GB
Total of 256 GB of RAM
Network: Infiniband
Not in www.top500.org!!!
Per node: Two Intel Xeon 5472 3 GHz Quad-Core Processors
DDR2-667 533 MHz RAM
Total of 544 GB of RAM
Network: Infiniband
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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)

What is the Main Source of Efficiency?

Answer: Reduced complexity of a fast algorithm is the main source of efficiency, NOT parallelization.

Nevertheless, parallelization is useful for reducing the CPU time and essential for memory usage.

Parallelization is necessary, but not sufficient.

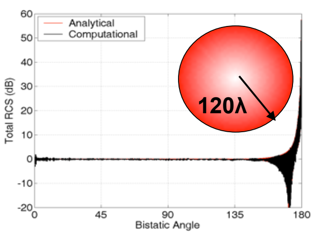
Dilemma: Faster algorithms with lower computational complexity require more complicated programming (ironic?), and hence they are much more difficult to parallelize.

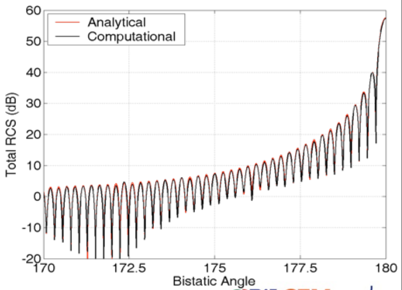
53 Million Unknowns

Sphere with radius of 120λ and diameter of 240λ

November 2007

53,112,384 Unknowns



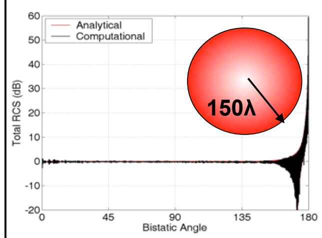


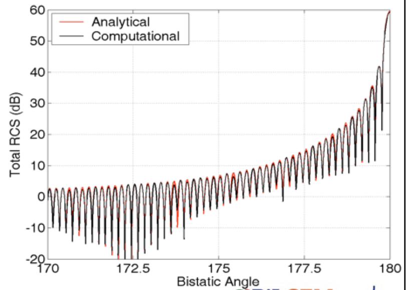
69 Million Unknowns

Sphere with radius of 150λ and diameter of 300λ

December 2007

69,177,600 Unknowns





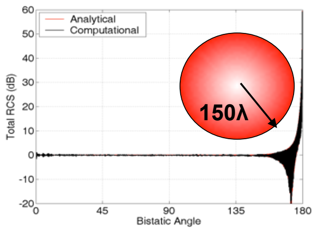
85 Million Unknowns

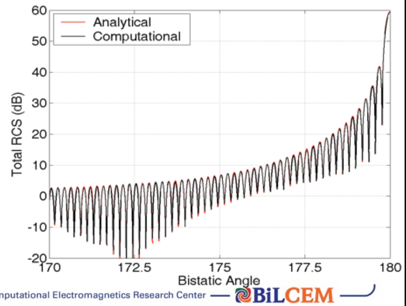
January 2008

Sphere with radius of 150λ and diameter of 300λ

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

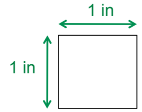
85,148,160 Unknowns





How Large are Large Matrix Equations?

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

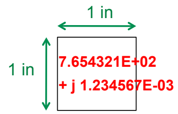


7.654321E+02
+ j 1.234567E-03

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

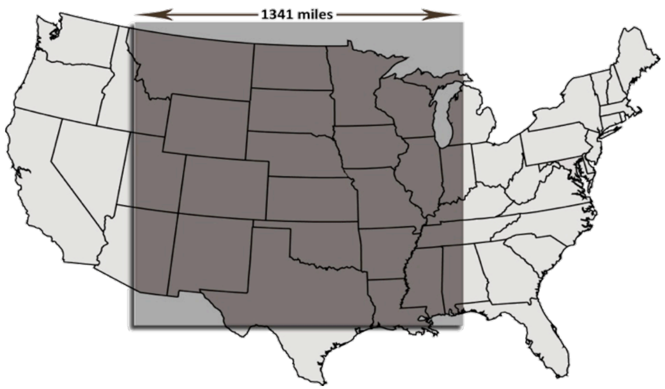
How Large are Large Matrix Equations?

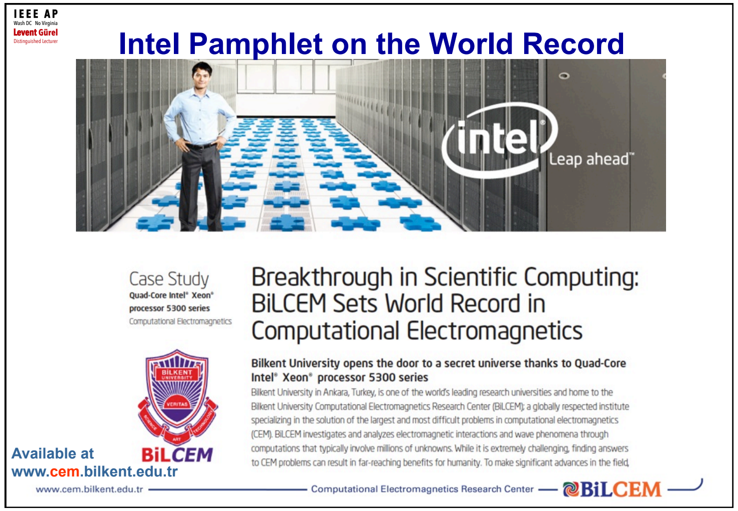
Each element of the matrix is a complex number with real and imaginary parts



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

85 Million × 85 Million Matrix





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Intel Pamphlet on the World Record
intel
Leap ahead
Case Study
Quad-Core Intel® Xeon® processor 5300 series
Computational Electromagnetics
Breakthrough in Scientific Computing: BiLCEM Sets World Record in Computational Electromagnetics
Bilkent University opens the door to a secret universe thanks to Quad-Core Intel® Xeon® processor 5300 series
Bilkent University in Ankara, Turkey, is one of the world's leading research universities and home to the Bilkent University Computational Electromagnetics Research Center (BiLCEM); a globally respected institute specializing in the solution of the largest and most difficult problems in computational electromagnetics (CEM). BiLCEM investigates and analyzes electromagnetic interactions and wave phenomena through computations that typically involve millions of unknowns. While it is extremely challenging, finding answers to CEM problems can result in far-reaching benefits for humanity. To make significant advances in the field,
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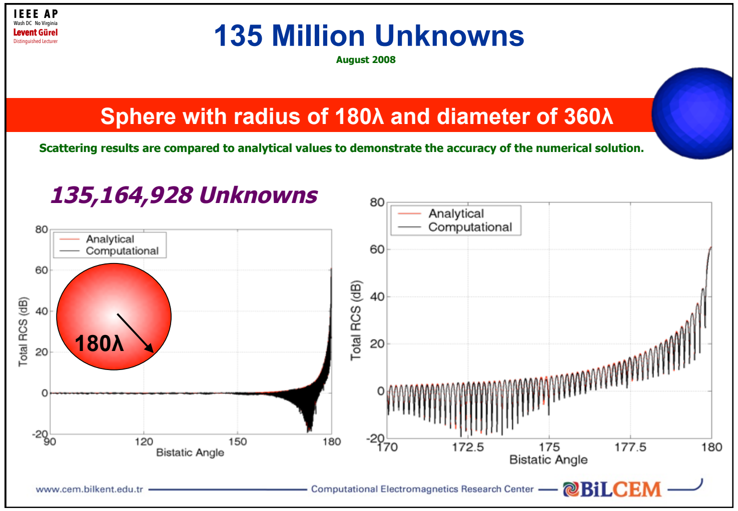

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135 Million Unknowns
August 2008
Sphere with radius of 180λ and diameter of 360λ
Scattering results are compared to analytical values to demonstrate the accuracy of the numerical solution.
135,164,928 Unknowns
Analytical
Computational
180λ
Total RCS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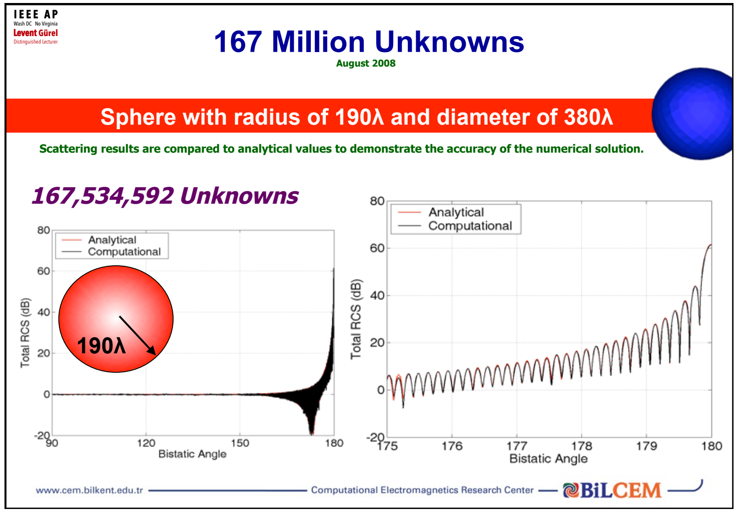

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167 Million Unknowns
August 2008
Sphere with radius of 190λ and diameter of 380λ
Scattering results are compared to analytical values to demonstrate the accuracy of the numerical solution.
167,534,592 Unknowns
Analytical
Computational
190λ
Total RCS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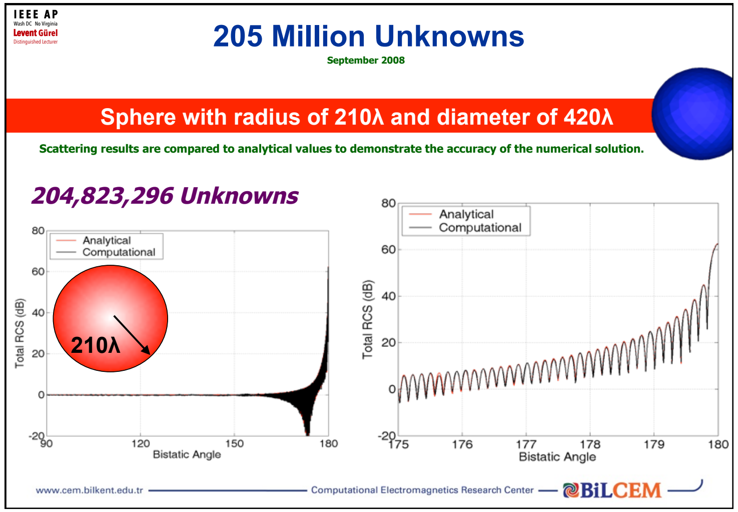

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205 Million Unknowns
September 2008
Sphere with radius of 210λ and diameter of 420λ
Scattering results are compared to analytical values to demonstrate the accuracy of the numerical solution.
204,823,296 Unknowns
Analytical
Computational
210λ
Total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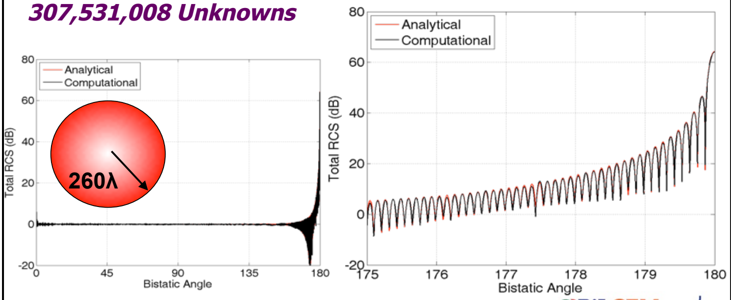
307 Million Unknowns

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



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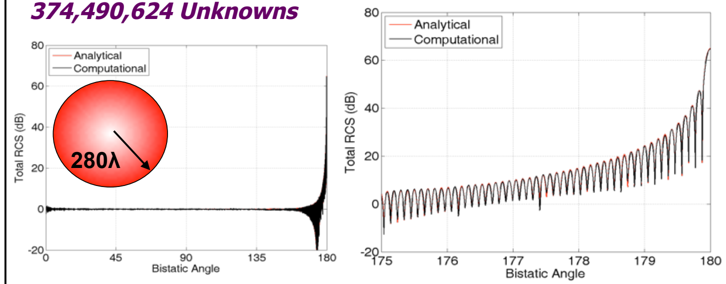
375 Million Unknowns

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



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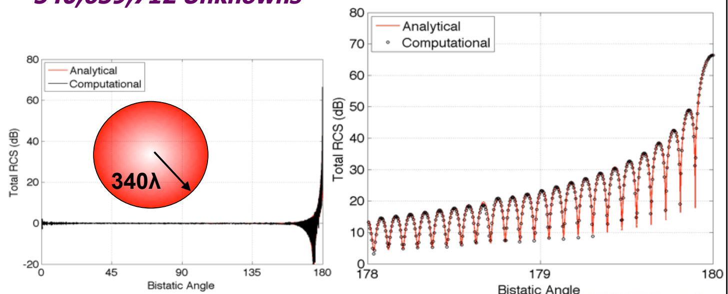
540 Million Unknowns

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



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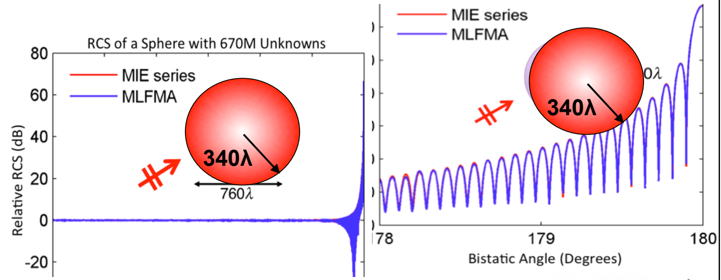
670 Million Unknowns

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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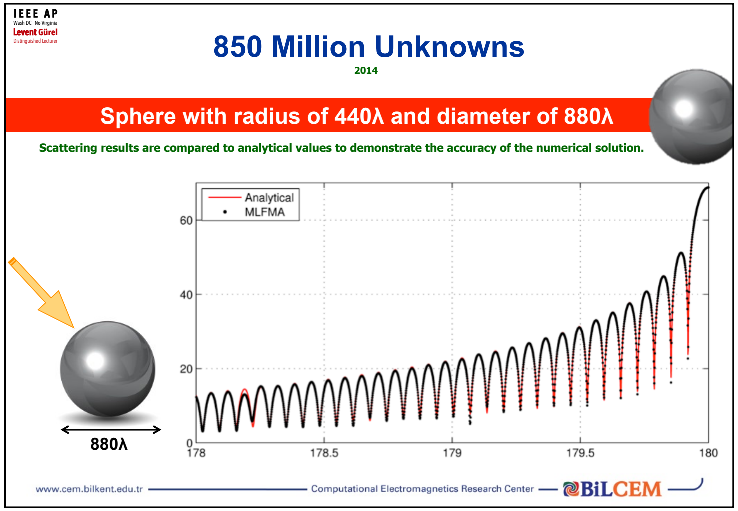
IEEE AP
Levent Gürel
850 Million Unknowns
2014
Sphere with radius of 440λ and diameter of 880λ
Scattering results are compared to analytical values to demonstrate the accuracy of the numerical solution.
Analytical
MLFMA
880λ
0
20
40
60
178
178.5
179
179.5
180
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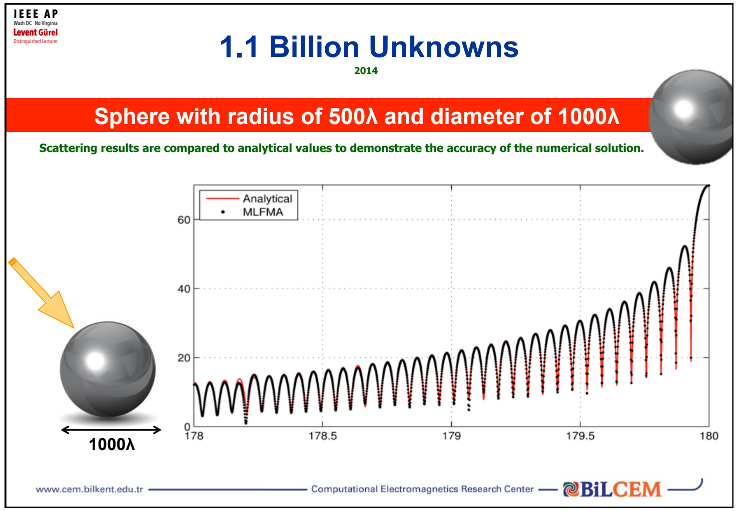
BiLCEM


IEEE AP
Levent Gürel
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.
Analytical
MLFMA
1000λ
0
20
40
60
178
178.5
179
179.5
180
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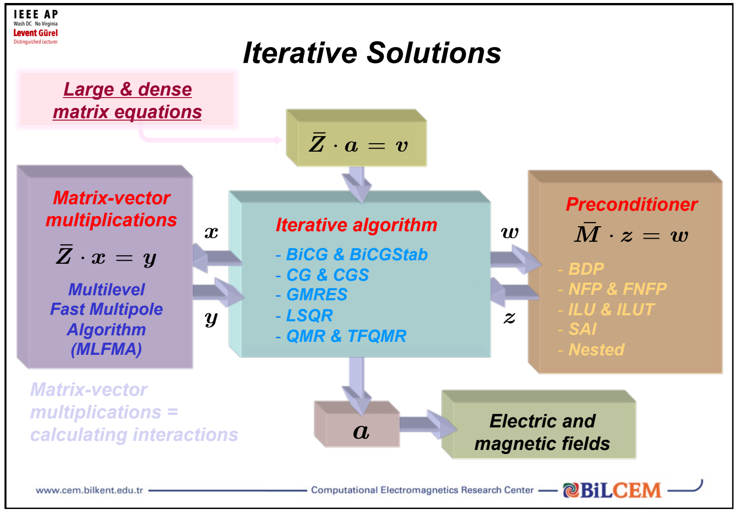
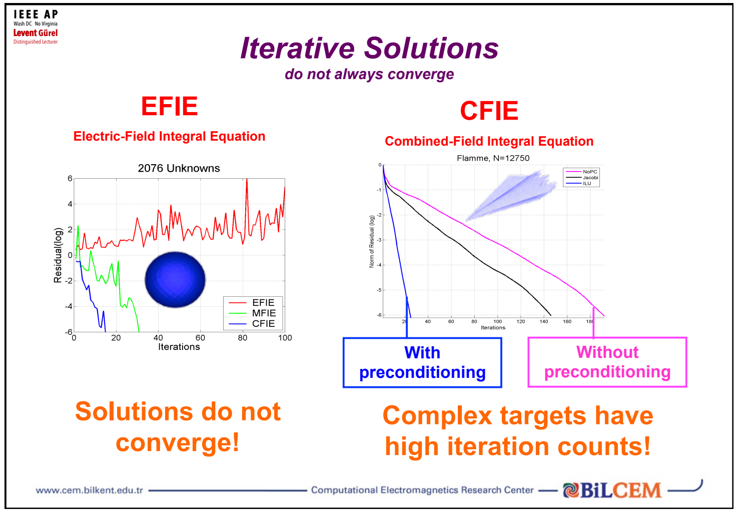
BiLCEM


IEEE AP
Levent Gürel
Iterative Solutions
Large & dense matrix equations
$\bar{Z} \cdot a = v$
Matrix-vector multiplications
$\bar{Z} \cdot x = y$
Multilevel Fast Multipole Algorithm (MLFMA)
x
y
Iterative algorithm
- BiCG & BiCGStab
- CG & CGS
- GMRES
- LSQR
- QMR & TFQMR
w
z
Preconditioner
$\bar{M} \cdot z = w$
- BDP
- NFP & FNFP
- ILU & ILUT
- SAI
- Nested
Matrix-vector multiplications = calculating interactions
a
Electric and magnetic fields
www.cem.bilkent.edu.tr
Computational Electromagnetics Research Center
BiLCEM


IEEE AP
Levent Gürel
Iterative Solutions
do not always converge
EFIE
Electric-Field Integral Equation
2076 Unknowns
Residual(log)
Iterations
EFIE
MFIE
CFIE
CFIE
Combined-Field Integral Equation
Flamme, N=12750
With preconditioning
Without preconditioning
Solutions do not converge!
Complex targets have high iteration counts!
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BiLCEM

Forward-Type Preconditioners

For the iterative solution of $\bar{Z} \cdot \boldsymbol{a} = \boldsymbol{v}$

find $\bar{M} \approx \bar{Z}$,

for which the solution of $\bar{M} \cdot \boldsymbol{z} = \boldsymbol{y}$ is cheap.

Then, solve $\bar{M}^{-1} \cdot \bar{Z} \cdot \boldsymbol{a} = \bar{M}^{-1} \cdot \boldsymbol{v}$

Iterative Solutions

require matrix-vector multiplications in the form of $\bar{Z} \cdot \boldsymbol{x}$.

Matrix-vector multiplication is provided by **MLFMA** in *O(NlogN)* time.

Only near-field interactions are stored:

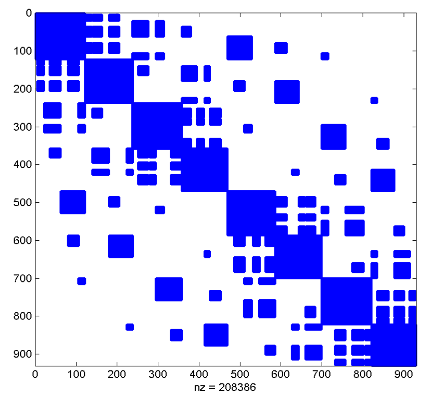
$$\bar{Z} \cdot \boldsymbol{x} = (\bar{Z}^{NF} + \bar{Z}^{FF}) \cdot \boldsymbol{x}$$

Sparse near-field matrix ($\bar{Z}^{NF}$)

Far-field interactions by MLFMA ($\bar{Z}^{FF}$)

$\bar{M} \approx \bar{Z}$ may be $\bar{Z}^{NF}$

Sparse Near-Field Matrix



Challenges and Requirements

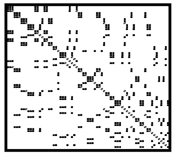
Challenges

- *System matrix is not readily available!*
- *Large linear systems!*
- *Indefinite systems!*

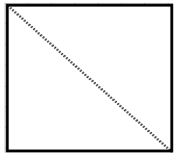
Requirements

- *Apply sparse preconditioning techniques*
- *O(NlogN) complexity (or lower)*
- *Parallelizable*

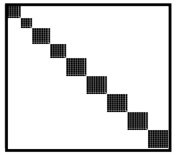
Simple Preconditioners



Filtered:
- Stronger elements in the impedance matrix are selected
- Adjustable size
- Difficult to factorize and use



Diagonal:
- Diagonal (self-unknown) elements in the impedance matrix are selected
- Size is fixed
- Easy to factorize and use



Block Diagonal:
- Block-diagonal (self-cluster) elements in the impedance matrix are selected
- Size is fixed
- Easy to factorize and use

Preconditioners (for MLFMA)

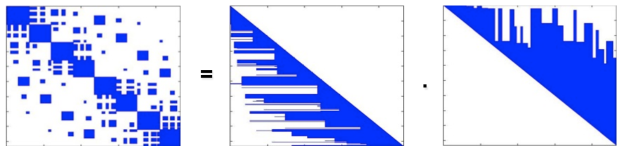
- *Near-Field Preconditioners*
- *Full-Matrix Preconditioners (Approximate)*
- *Schur Preconditioners for Dielectric Formulations*

Sparse Near-Field Preconditioners

- LU (too expensive)
- ILU: Incomplete LU
- SAI: Sparse Approximate Inverse
- INF: Iterative Near-Field Preconditioner

Alternatively: Use more than the available near-field matrix

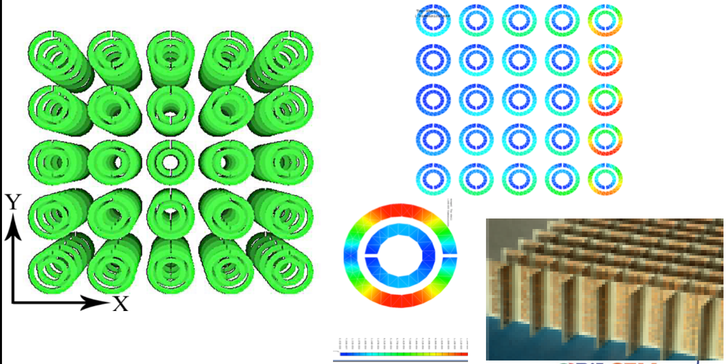
Inverse of a Sparse Matrix is NOT Sparse!



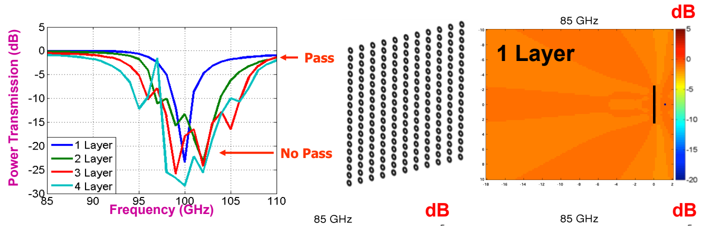
$\bar{Z}^{NF}$ $\bar{L}$ $\bar{U}$

$$\bar{Z}^{NF} = \bar{L}\cdot\bar{U}, \qquad x = \left(\bar{L}\cdot\bar{U}\right)^{-1}\cdot y$$

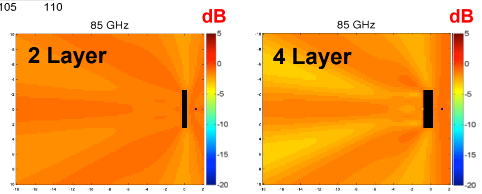
Metamaterials
Split-Ring Resonators



SRR Walls

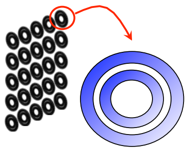


Meta Property:
Stop band in frequency!



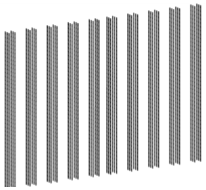
Special Configurations

Closed-Ring Resonators (CRRs)



All pass!

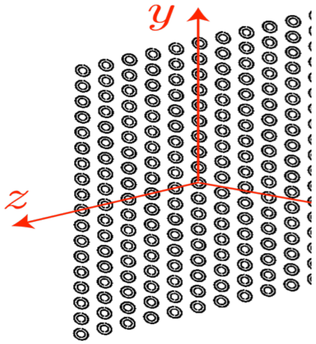
Thin Wire Array (TWA)



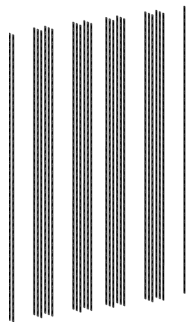
No pass!

Composite Metamaterial (CMM)

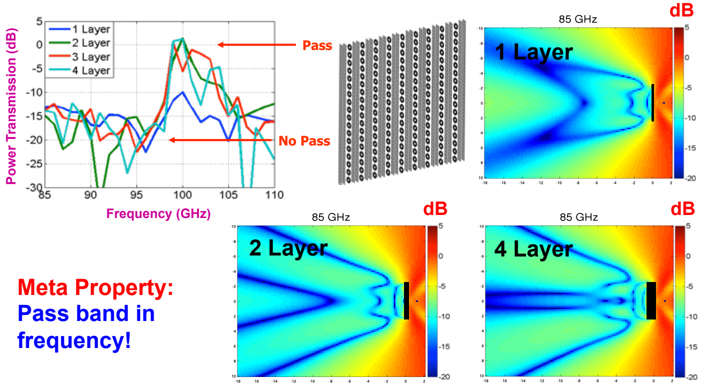
Split-Ring Resonators (SRRs)



Thin Wire Array (TWA)



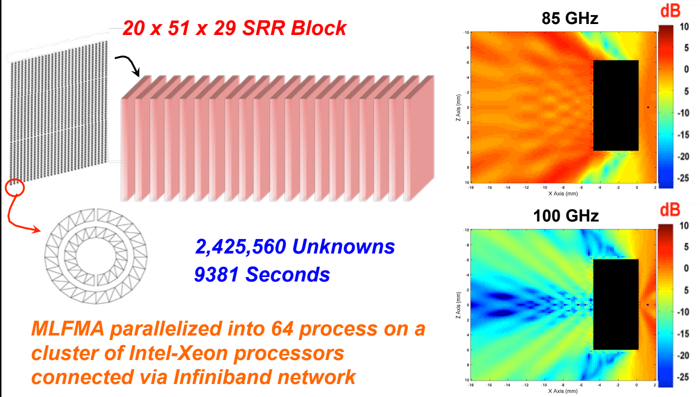
CMM Walls



Meta Property:
Pass band in frequency!

Large MM Problem

20 x 51 x 29 SRR Block

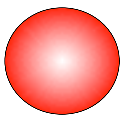


2,425,560 Unknowns
9381 Seconds

MLFMA parallelized into 64 process on a cluster of Intel-Xeon processors connected via Infiniband network

BENCHMARKING

Available from
www.cem.bilkent.edu.tr

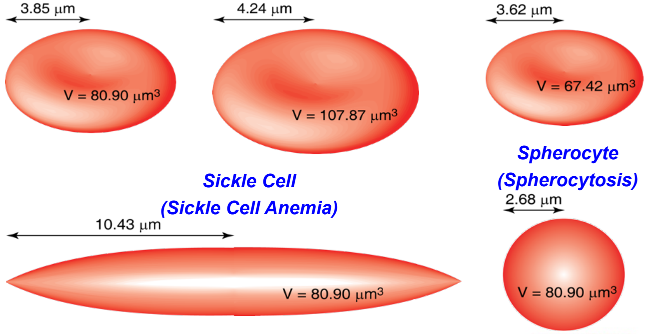


Scattering from sphere (radius: 20λ - 340λ)
Web-based application: Upload the computational results and get the error with respect to analytical Mie-series solutions.

Scattering from NASA Almond (size: 94λ - 1514λ)
*Web-based application: Upload the computational results and get the error with respect to **our** results.*

WEB-BASED BENCHMARKING TOOL

Red Blood Cells (RBCs)



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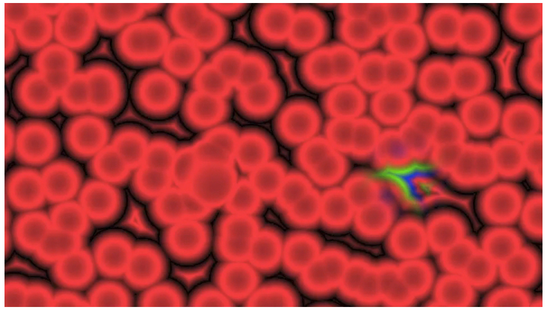
Distinguished Lecturer

Red Blood Cells (RBCs)



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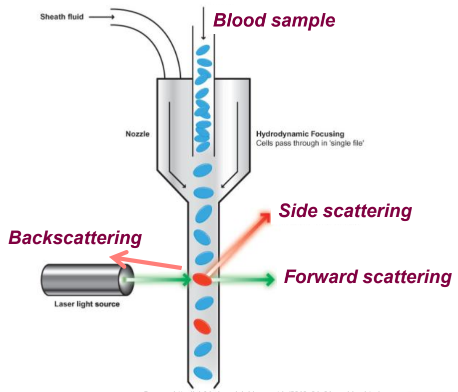
Flow Cytometry



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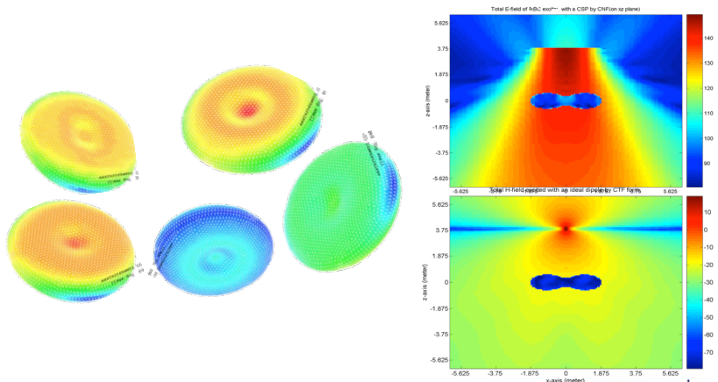
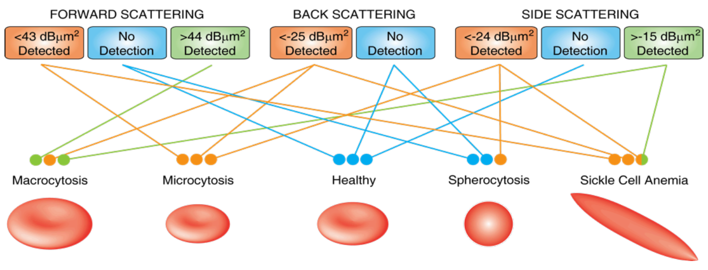
Scattering from and Imaging of Red Blood Cells



Decision Chart



Multi-Disciplinary Approach