2015 URSI Commission B School
for Young Scientists

Integral Equations, Fast Algorithms, and Parallelization Strategies for the Solution of Extremely Large Problems in Computational Electromagnetics

Lecture Notes

May 17, 2015

ExpoMeloneras Convention Centre

Gran Canaria, Spain

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* This School is organized during the "2015 URSI Atlantic Radio Science Conference" (URSI AT-RASC 2015), May 16-24, 2015, Gran Canaria, Spain.

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Preface

The “2015 URSI Commission B School for Young Scientists” is organized by URSI Commission B and is arranged on the occasion of the “2015 URSI Atlantic Radio Science Conference” (URSI AT-RASC 2015), May 16-24, 2015, Gran Canaria, Spain. This School is a one-day event held during URSI AT-RASC 2015, and is sponsored jointly by URSI Commission B and the URSI AT-RASC 2015 Organizing Committee. The School offers a short, intensive course, where a series of lectures will be delivered by a leading scientist in the Commission B community. Young scientists are encouraged to learn the fundamentals and future directions in the area of electromagnetic theory from these lectures.

Program

1. Course Title

Integral Equations, Fast Algorithms, and Parallelization Strategies for the Solution of Extremely Large Problems in Computational Electromagnetics

2. Course Instructor

Prof. Levent Gurel
CEO, ABAKUS Computing Technologies, Turkey;
Adjunct Professor, ECE, University of Illinois at Urbana-Champaign, USA

3. Course Program

Lecture 1

- Date and Time: 9:00-13:00, Sunday, May 17, 2015
- Venue: ExpoMeloneras Convention Centre, Gran Canaria, Spain
- Lecture Topics:

  Introduction
  Computational electromagnetics
  Maxwell's equations
  Integral equations
  Method of moments
  Fast multipole method (FMM)
  Clustering, aggregation, translation, and disaggregation
  Complexity of FMM
  Multilevel fast multipole algorithm (MLFMA)
  Recursive clustering and tree structure
  Interpolation and anterpolation
  Multilevel aggregation, translation, and disaggregation
  Complexity of MLFMA

Lecture 2

- Date and Time: 14:00-18:00, Sunday, May 17, 2015
- Venue: ExpoMeloneras Convention Centre, Gran Canaria, Spain
- Lecture Topics:

  Parallelization of MLFMA
  Load balancing
  Simple parallelization
  Hybrid parallelization
  Hierarchical parallelization
  Iterative methods
  Preconditioners
  Solution of large problems
  Application examples
  Conclusions

Lecture Abstract

Integral Equations, Fast Algorithms, and Parallelization Strategies for the Solution of Extremely Large Problems in Computational Electromagnetics

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Professor Emeritus, Bilkent University, Turkey
Founder, Computational Electromagnetics Research Center (BiLCEM)
Email: lgurel@gmail.com

2015 edition of the *URSI Commission B School for Young Scientists* lectures by Prof. Levent Gurel focuses on the solution of extremely large problems in electromagnetics. Fast solvers, such as the fast multipole method (FMM) and the multilevel fast multipole algorithm (MLFMA), will be considered. These methods can be applied to scattering, radiation, propagation, resonance, guidance, and transmission problems in electromagnetics. Furthermore, they can also be applied to the solution of problems from other disciplines, such as quantum mechanics, astrophysics, molecular dynamics, etc. Wave phenomena in electrodynamics, acoustics, elastics and seismic problems can be studied with these methods. As such, applications can be derived from a very wide portfolio, including, but not limited to optics, nanotechnology, metamaterials, antennas, radars, remote sensing, imaging, biomedical, bioelectromagnetics, stealth technology and radar-cross-section (RCS) computations.

Following a general introduction to computational electromagnetics, this course focuses on the fast and accurate solutions of large-scale electromagnetic modeling problems involving three-dimensional geometries with arbitrary shapes using FMM, MLFMA, and parallel MLFMA. Accurate simulations of real-life electromagnetics problems with integral equations require the solution of dense matrix equations involving millions of unknowns. Solutions of those extremely large problems cannot be achieved easily, even when using the most powerful computers with state-of-the-art technology. Nevertheless, some of the world's largest integral-equation problems in computational electromagnetics can be solved by employing fast algorithms implemented on parallel computers. Most recently, we have achieved the solution of 1,000,000,000x1,000,000,000 (one billion!) dense matrix equations! This achievement requires a multidisciplinary study involving physical understanding of electromagnetics problems, novel parallelization strategies, constructing parallel clusters, advanced mathematical methods for integral equations, fast solvers, iterative methods, preconditioners, and linear algebra. In this course, various examples of CEM problems derived from real-life applications are considered.

Biographical Sketch of Course Instructor

Levent Gürel received the B.Sc. degree from the Middle East Technical University (METU) in 1986, and the M.S. and Ph.D. degrees from the University of Illinois at Urbana-Champaign (UIUC) in 1988 and 1991, respectively, in electrical and computer engineering. After spending 3 years at the Thomas. J. Watson Research Center of IBM in Yorktown Heights, New York, where he worked on the solution of electromagnetics problems relevant to the computer industry, he moved to Bilkent University, Ankara, Turkey. During his 20 years with Bilkent University (1994-2014), he served as the Founding Director of the Computational Electromagnetics Research Center (BiLCEM) and a professor of electrical engineering. Currently, Prof. Gürel is the Founder and CEO of the ABAKUS Computing Technologies company that is geared towards providing advanced solutions and creating cutting-edge technologies through R&D projects in computational sciences. He is also an adjunct professor at the Electrical and Computer Engineering Department of UIUC, a consultant to industry, and a member of the Board of Trustees of Izmir University of Economics.

Prof. Gürel is named an IEEE Distinguished Lecturer for 2011-2014. In 2013, his contributions to science have been recognized by the Electrical and Computer Engineering Department of the University of Illinois with the Distinguished Alumni Award.

Prof. Gürel was named an IEEE Fellow "on the basis of his contributions to fast methods and algorithms for computational electromagnetics" in 2009. Also, he was elevated to the Fellow grade by the Electromagnetics Academy in 2007 and elected to become a Fellow of the Applied Computational Electromagnetic Society (ACES) in 2011. He received two prestigious awards from the Turkish Academy of Sciences (TUBA) in 2002 and the Scientific and Technical Research Council of Turkey (TUBITAK) in 2003. He served as a member of the ACES Board of Directors during 2011-2014.

He has been organizing and serving as the General Chairman and Editor of the biennial Computational Electromagnetics International Workshops held in 2007-2015. Since 2003, Prof. Gürel has been serving as an associate editor for Radio Science, IEEE Antennas and Wireless Propagation Letters, IET Microwaves, Antennas & Propagation, JEMWA, PIER, ACES Journal, and ACES Express.

Prof. Gürel was invited to address the 2011 ACES Conference as a Plenary Speaker and a TEDx conference in 2014. He served as the Chairman of the AP/MTT/ED/EMC Chapter of the IEEE Turkey Section in 2000-2003. He founded the IEEE EMC Chapter in Turkey in 2000. He served as the Cochairman of the 2003 IEEE International Symposium on Electromagnetic Compatibility.

Integral Equations, Fast Algorithms, and Parallelization Strategies for the Solution of Extremely Large Problems in Computational Electromagnetics

May 17, 2015

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CEO, ABAKUS Computing Technologies, Turkey;

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Integral Equations, Fast Algorithms, and Parallelization Strategies

for the Solution of Extremely Large Problems

in Computational Electromagnetics

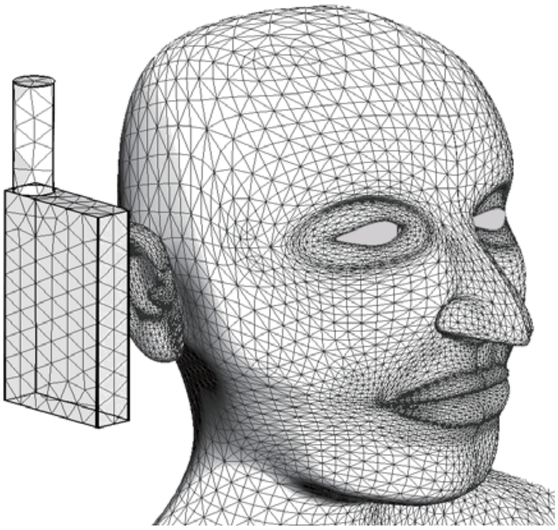
Prof. Levent Gürel

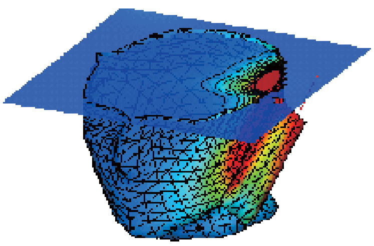
CEO, ABAKUS Computing Technologies

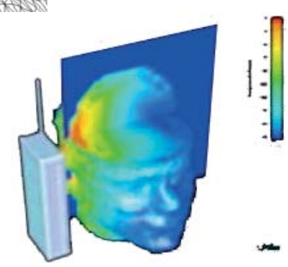
Adjunct Professor, ECE, Univ. of Illinois at Urbana-Champaign

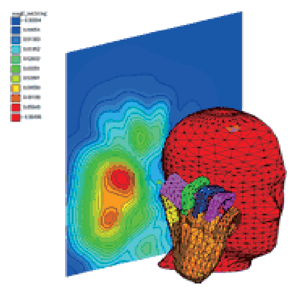
May 2015

Radiation into Living Organisms









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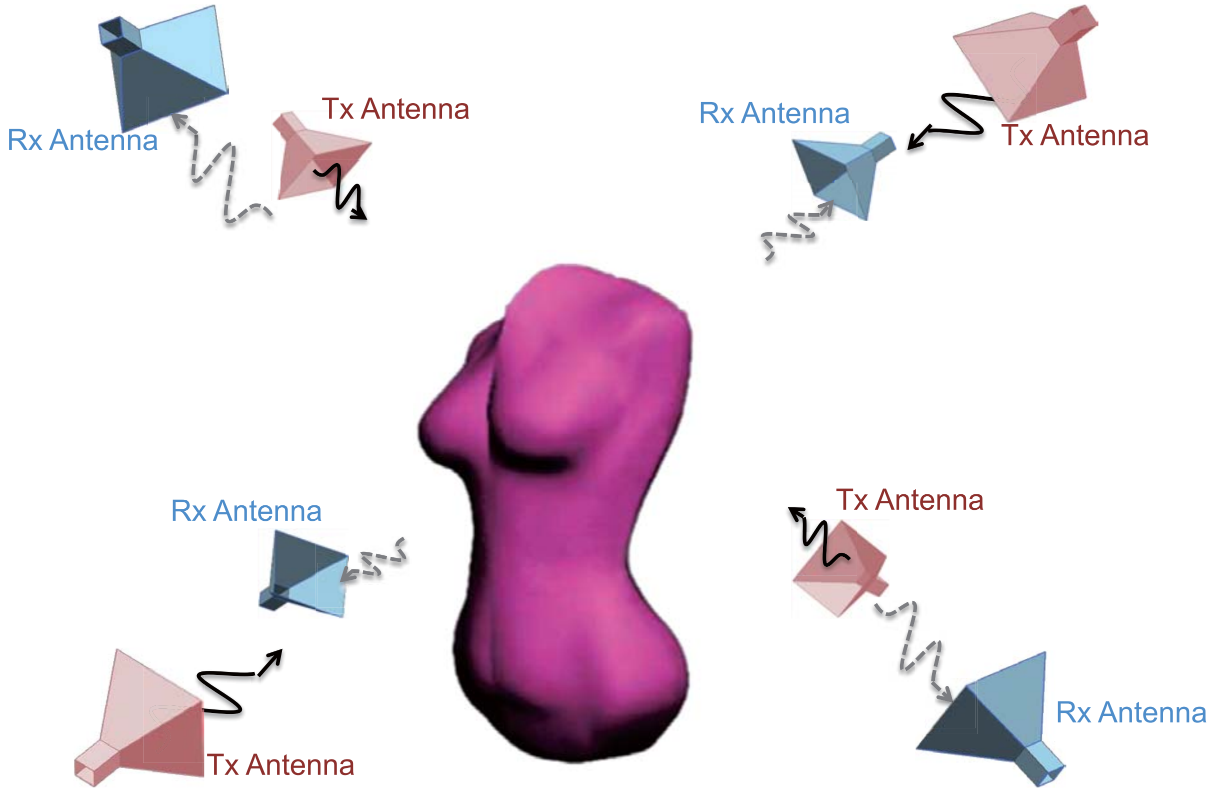
Microwave Imaging



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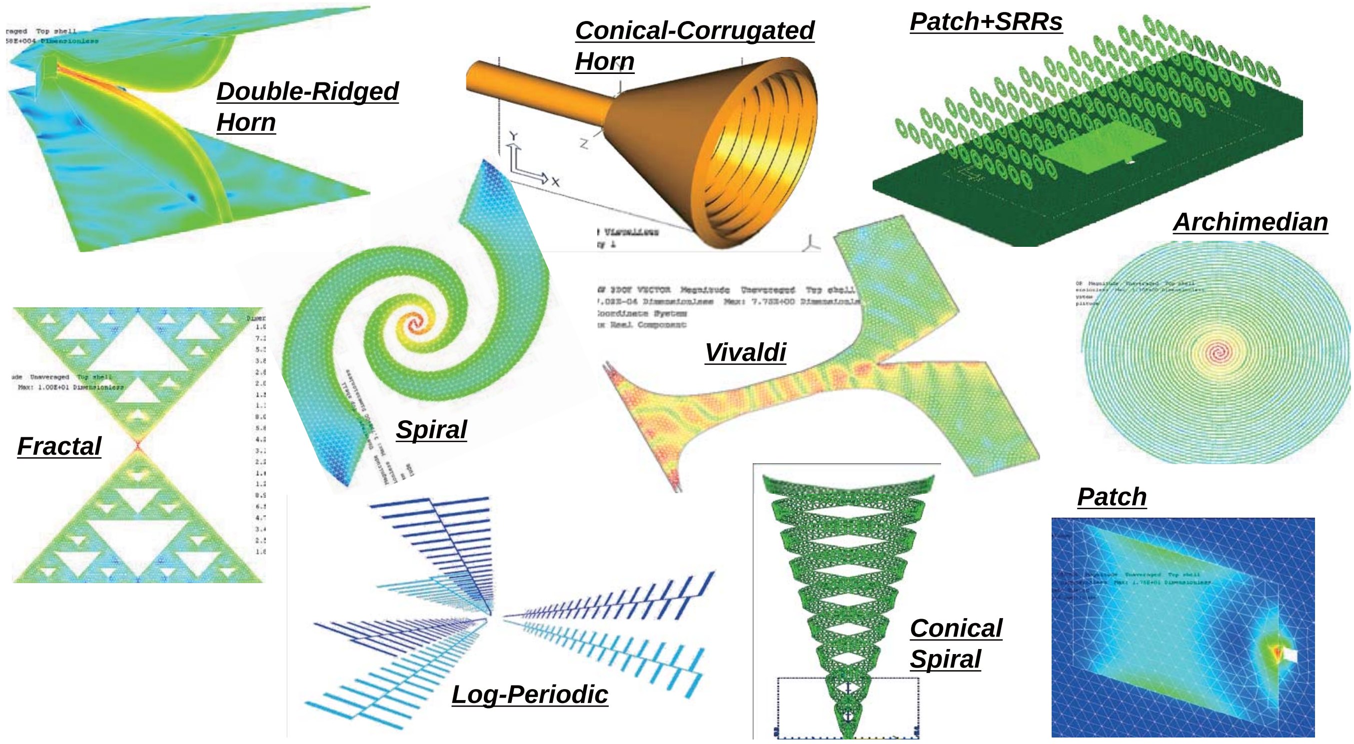
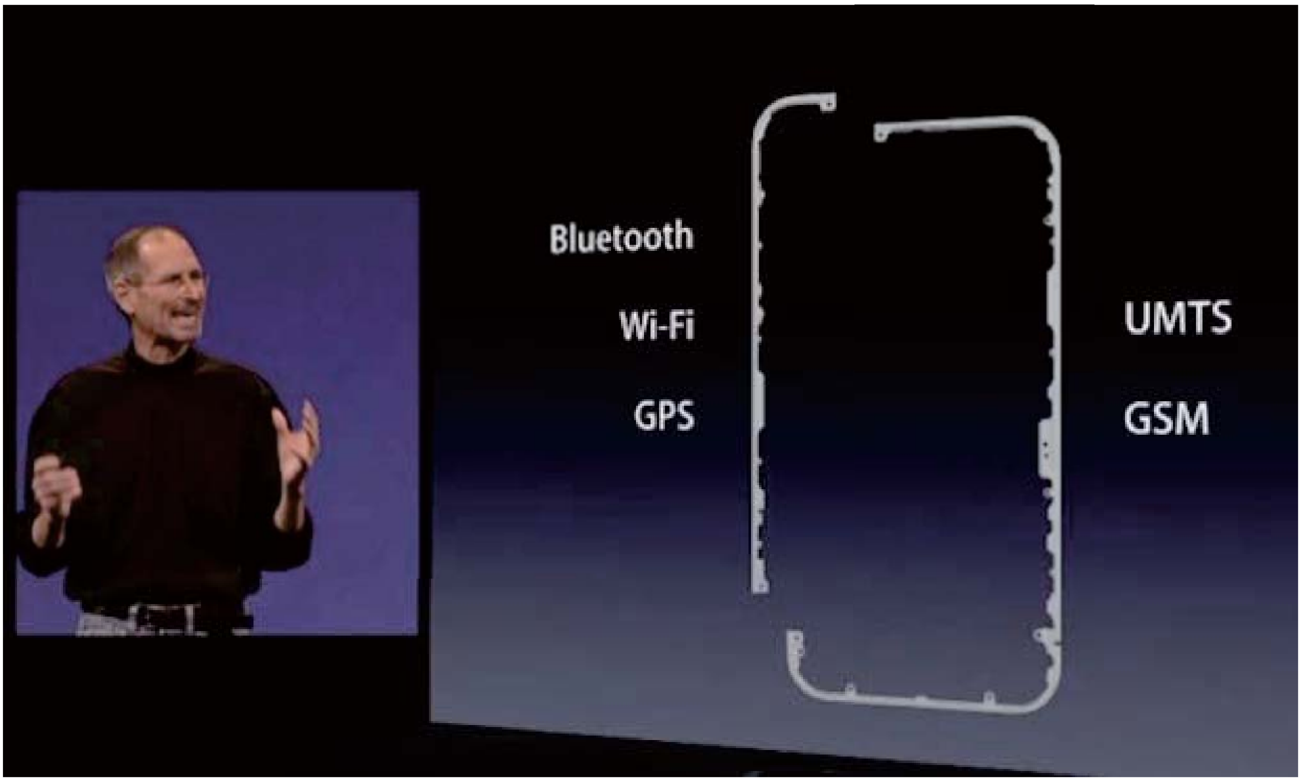
Antennas

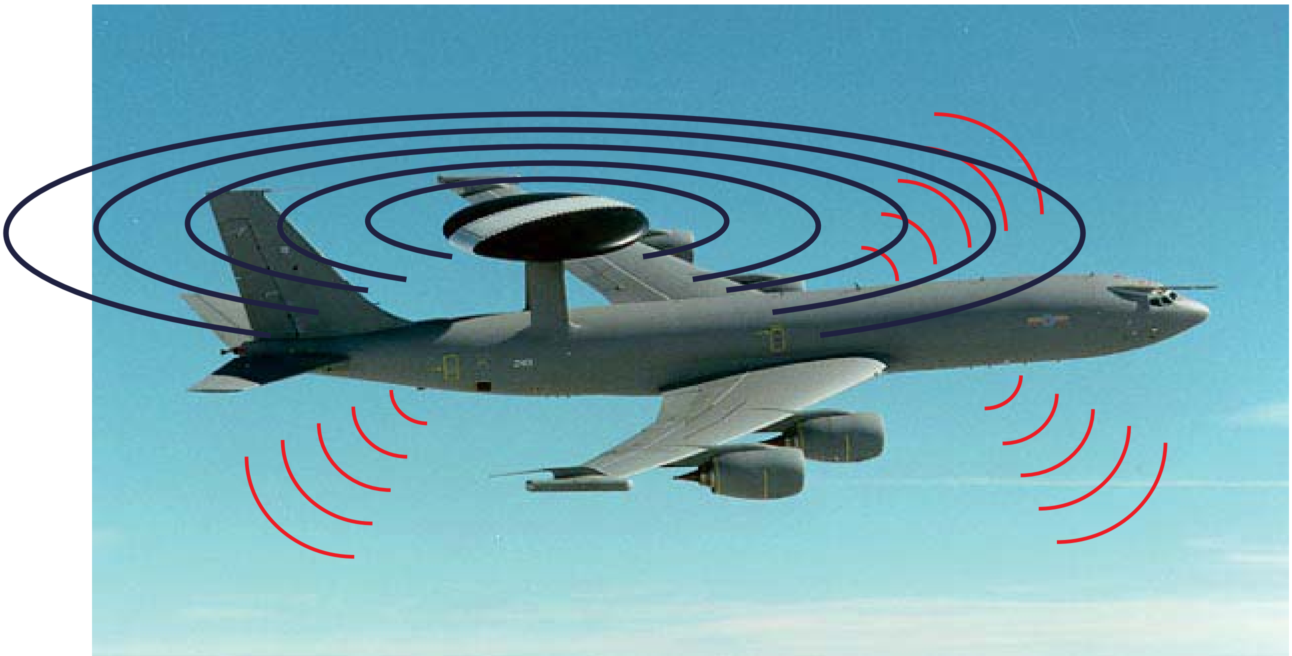


Mobile Device Antennas



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

Maxwell's Equations

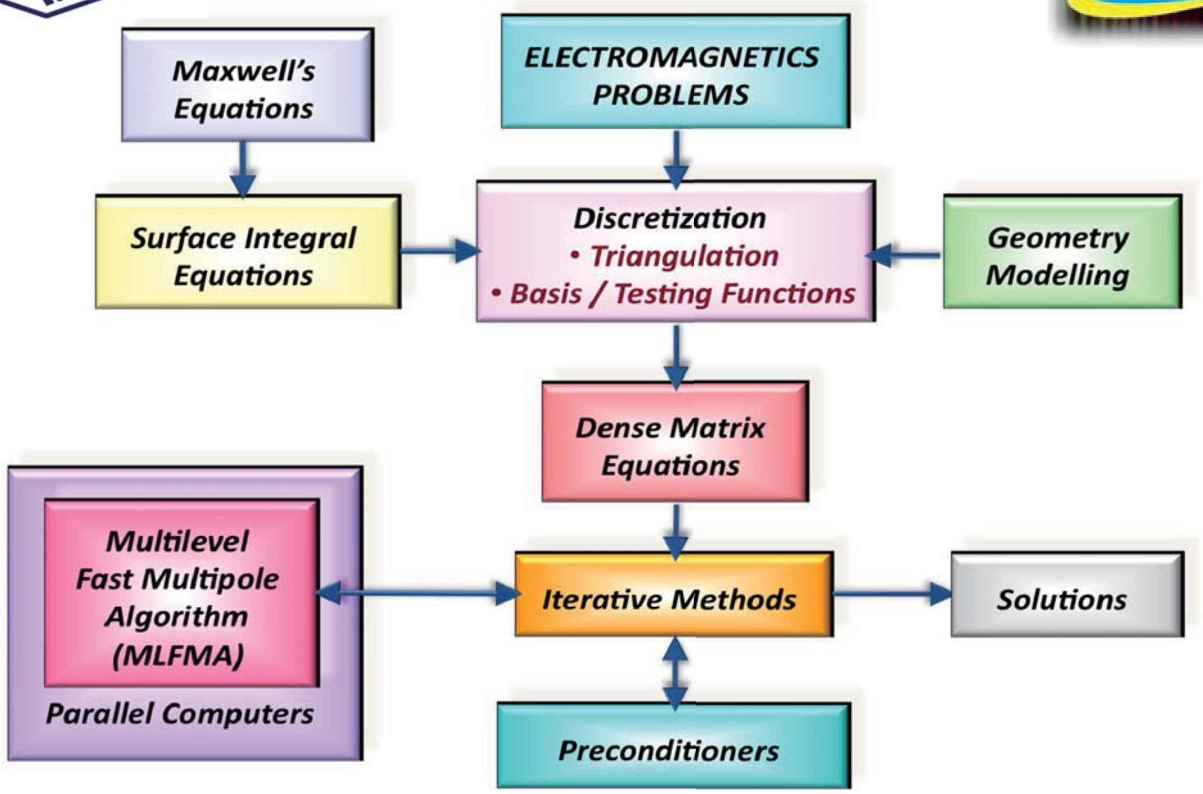
$$\nabla \times \bar{E}(\bar{r},t) = -\frac{\partial}{\partial t}\bar{B}(\bar{r},t)$$

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

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

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

Simulation Environment



Surface Integral Equations

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

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

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

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

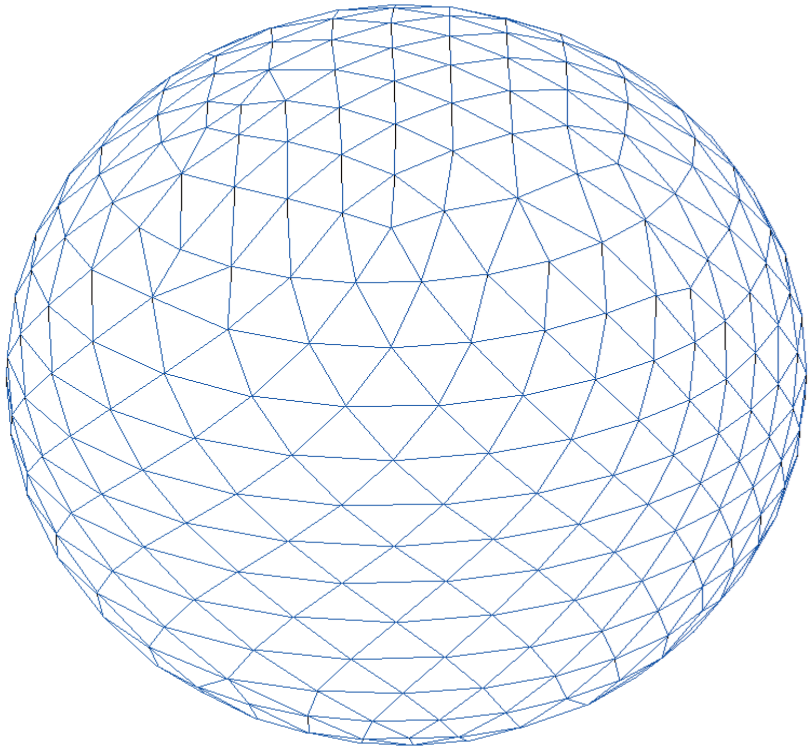
- *Combined-Field Integral Equation (CFIE):*

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

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

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

Geometry Discretization



Mesh Size: λ/10

Current Discretization (Expansion)

Number of unknowns

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

Basis functions

Discretization of EFIE

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

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

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

- Matrix equation:

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

Basis functions

Testing functions

- Matrix elements:

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

Discretization of MFIE

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

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

- Matrix equation:

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

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

Basis functions

- Matrix elements:

Testing functions

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

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CFIE
Combined-Field Integral Equation

- Matrix elements:

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

- Matrix equation:

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

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Matrix Elements…

…are electromagnetic interactions

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

Testing functions

Basis functions

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

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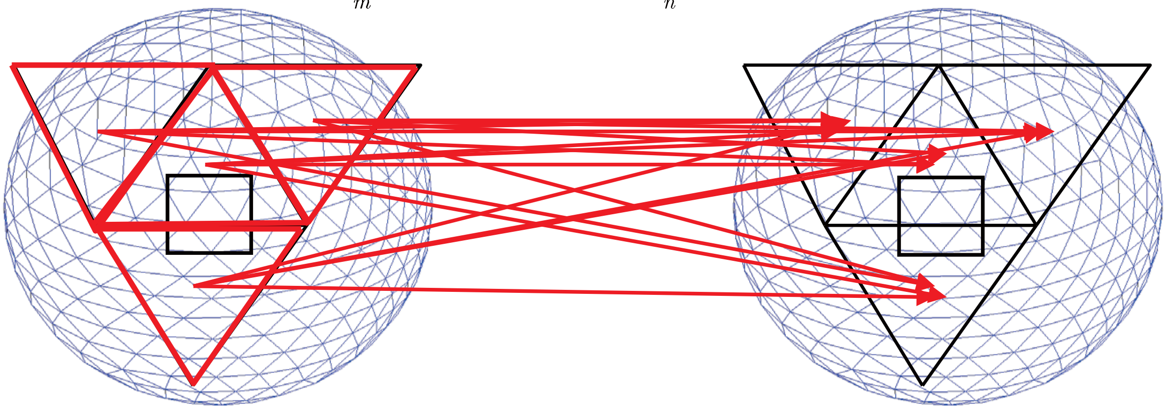
MOM Interactions

- MOM: Perform interactions one by one (for each basis and testing functions):

$$\sum_{n=1}^{N} Z_{mn}^{M} a_n = -\int_{S_m} d\boldsymbol{r}\,\boldsymbol{t}_m(\boldsymbol{r}) \cdot \hat{\boldsymbol{n}} \times \int_{S_n} d\boldsymbol{r}'\boldsymbol{b}_n(\boldsymbol{r}') \times \nabla' g(\boldsymbol{r},\boldsymbol{r}')\, a_n$$



- Basis domain
- Testing domain

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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*

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

Matrix-Vector Multiplications

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

x

y

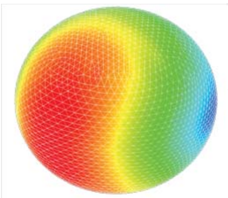
Iterative Algorithm

w

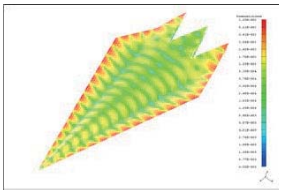
z

Preconditioner

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



a



Iterative Solutions

- *Large matrix equations*

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

Parallel Multilevel Fast Multipole Algorithm (MLFMA)

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

x

y

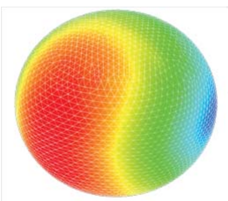
- **CG and CGS**
- **BiCG and BiCGStab**
- **QMR and TFQMR**
- **GMRES**
- **LSQR**

w

z

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

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



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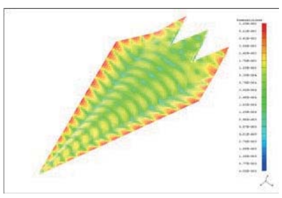

Fast Multipole Method (FMM)

Prof. Levent Gürel
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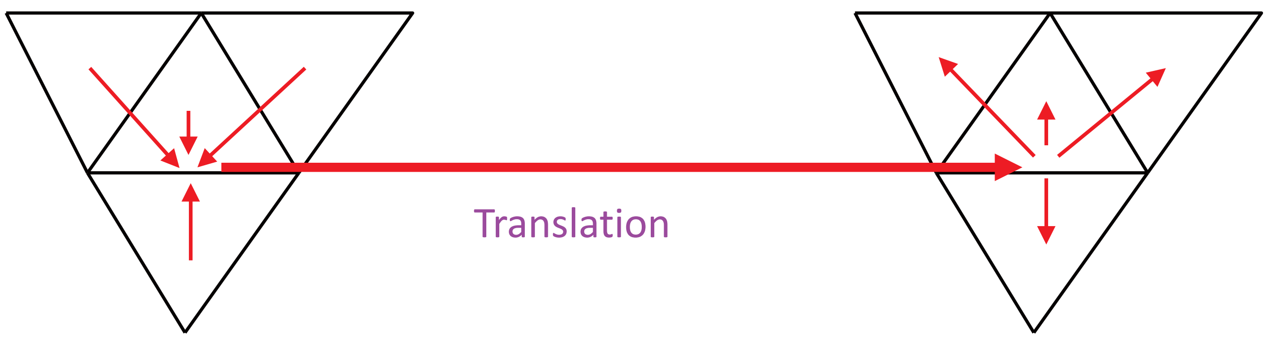
Adjunct Professor, ECE, Univ. of Illinois at Urbana-Champaign

May 2015

Fast Multipole Method (FMM)

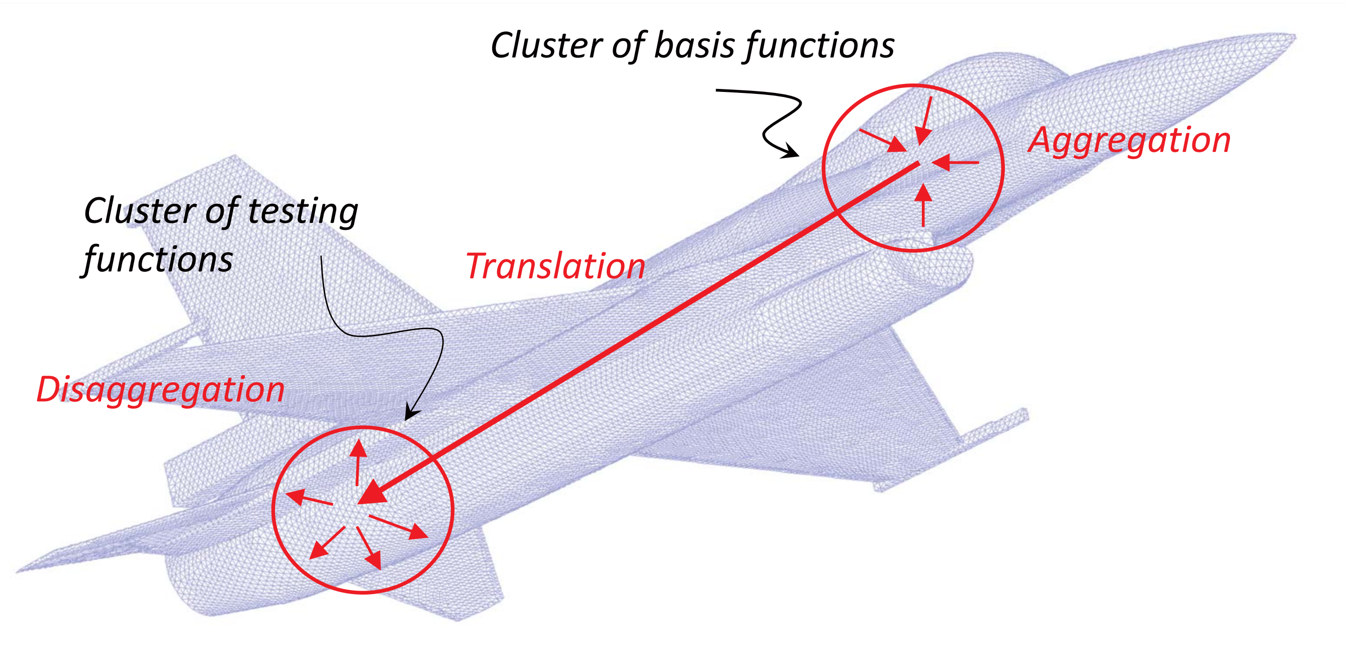
- FMM: Perform matrix-vector multiplications (for the iterative method) by using the factorization of the Green's function.

- Calculate the interactions in group-by-group manner:



- Basis domain
- Testing domain

Fast Multipole Method



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

Fast Multipole Method

$$g(\boldsymbol{r},\boldsymbol{r'}) = \frac{e^{ik|\boldsymbol{r}-\boldsymbol{r'}|}}{4\pi|\boldsymbol{r}-\boldsymbol{r'}|} = \frac{e^{ik|\boldsymbol{D}+\boldsymbol{d}|}}{|\boldsymbol{D}+\boldsymbol{d}|}$$

Factorize the Green's Function:

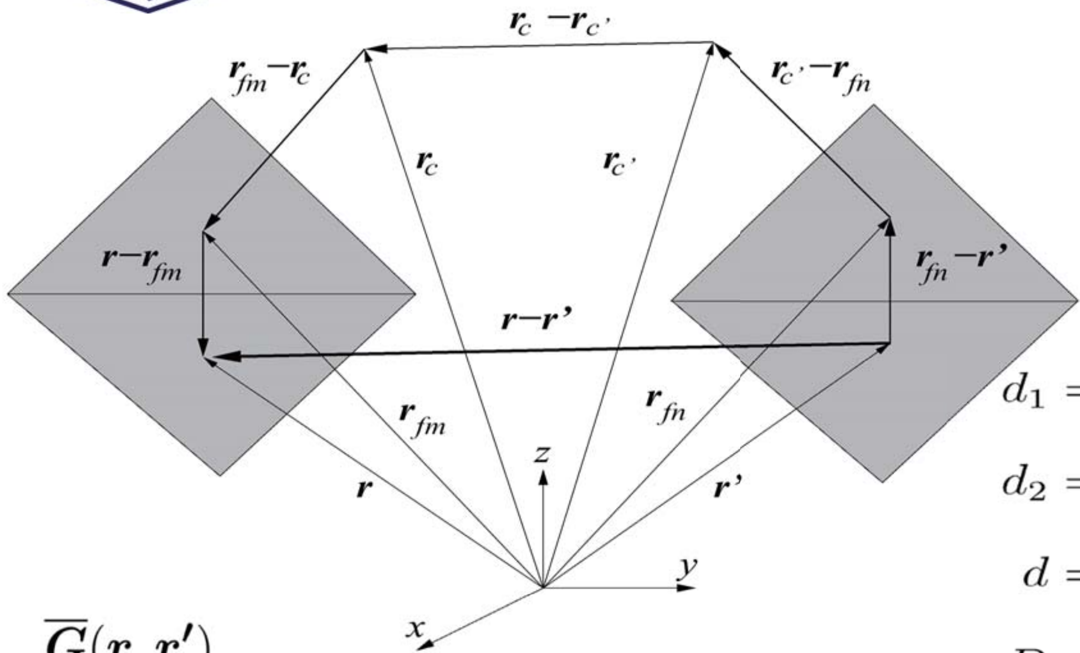
$$\frac{e^{ik|\boldsymbol{D}+\boldsymbol{d}|}}{4\pi|\boldsymbol{D}+\boldsymbol{d}|} = \frac{ik}{4\pi}\sum_{l=0}^{\infty}(-1)^l(2l+1)j_l(kd)h_l^{(1)}(kD)P_l(\hat{\boldsymbol{d}}\cdot\hat{\boldsymbol{D}}) \quad d < D$$

Using the identity: $$4\pi i^l j_l(kd)P_l(\hat{\boldsymbol{d}}\cdot\hat{\boldsymbol{D}}) = \int d^2\hat{\boldsymbol{k}}e^{i\boldsymbol{k}\cdot\boldsymbol{d}}P_l(\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{D}})$$

Rewrite it: $$\boxed{\frac{e^{ik|\boldsymbol{D}+\boldsymbol{d}|}}{4\pi|\boldsymbol{D}+\boldsymbol{d}|} \approx \frac{1}{4\pi}\int d^2\hat{\boldsymbol{k}}e^{i\boldsymbol{k}\cdot\boldsymbol{d}}T_L(k,D,\theta)}$$

$$T_L(k,D,\theta) = \frac{ik}{4\pi}\sum_{l=0}^{L} i^l(2l+1)h_l^{(1)}(kD)P_l(cos\theta)$$

FMM: Evaluating the Interactions



$$d_1 = \boldsymbol{r}_{rfm} + \boldsymbol{r}_{fmc}$$

$$d_2 = \boldsymbol{r}_{c'fn} + \boldsymbol{r}_{fnr'}$$

$$d = d_1 + d_2$$

$$D = \boldsymbol{r}_{cc'}$$

$$\overline{\boldsymbol{G}}(\boldsymbol{r}, \boldsymbol{r}')$$

$$\approx \frac{1}{4\pi} \int d^2\hat{\boldsymbol{k}} (\overline{\boldsymbol{I}} - \hat{\boldsymbol{k}}\hat{\boldsymbol{k}}) e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_{rfm} + \boldsymbol{r}_{fmc} + \boldsymbol{r}_{c'fn} + \boldsymbol{r}_{fnr'})} T_L(k, |\boldsymbol{r}_{cc'}|, \hat{\boldsymbol{r}}_{cc'} \cdot \hat{\boldsymbol{k}})$$

FMM: Evaluating the Interactions

EFIE

$$Z^E_{mn} = \frac{1}{4\pi} \int d^2\hat{\boldsymbol{k}} \boldsymbol{F}^E_{fmc}(\hat{\boldsymbol{k}}) T_L(k, |\boldsymbol{r}_{cc'}|, \hat{\boldsymbol{r}}_{cc'} \cdot \hat{\boldsymbol{k}}) \cdot \boldsymbol{F}^E_{fnc'}(\hat{\boldsymbol{k}})$$

MFIE

$$Z^M_{mn} = \frac{k}{4\pi i} \int d^2\hat{\boldsymbol{k}} \boldsymbol{F}^M_{fmc}(\hat{\boldsymbol{k}}) T_L(k, |\boldsymbol{r}_{cc'}|, \hat{\boldsymbol{r}}_{cc'} \cdot \hat{\boldsymbol{k}}) \cdot \boldsymbol{F}^M_{fnc'}(\hat{\boldsymbol{k}})$$

EFIE

$$\boldsymbol{F}^E_{fmc}(\hat{\boldsymbol{k}}) = e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_{fm} - \boldsymbol{r}_c)} \int_{S_m} d\boldsymbol{r} e^{i\boldsymbol{k}\cdot(\boldsymbol{r} - \boldsymbol{r}_{fm})} (\overline{\boldsymbol{I}} - \hat{\boldsymbol{k}}\hat{\boldsymbol{k}}) \cdot \boldsymbol{t}_m(r)$$

$$\boldsymbol{F}^E_{fnc'}(\hat{\boldsymbol{k}}) = e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_{c'} - \boldsymbol{r}_{fn})} \int_{S_n} d\boldsymbol{r}' e^{-i\boldsymbol{k}\cdot(\boldsymbol{r}' - \boldsymbol{r}_{fn})} (\overline{\boldsymbol{I}} - \hat{\boldsymbol{k}}\hat{\boldsymbol{k}}) \cdot \boldsymbol{b}_n(\boldsymbol{r}')$$

MFIE

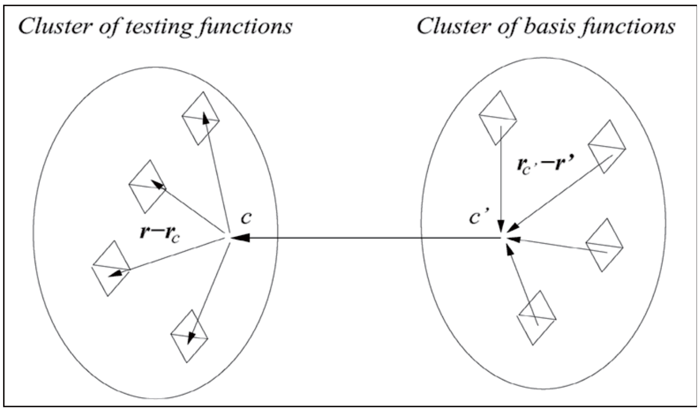
$$\boldsymbol{F}^M_{fmc}(\hat{\boldsymbol{k}}) = -\hat{\boldsymbol{k}} \times e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_{fm} - \boldsymbol{r}_c)} \int_{S_m} d\boldsymbol{r} e^{i\boldsymbol{k}\cdot(\boldsymbol{r} - \boldsymbol{r}_{fm})} \boldsymbol{t}_m(r) \times \hat{\boldsymbol{n}}$$

$$\boldsymbol{F}^M_{fnc'}(\hat{\boldsymbol{k}}) = e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_{c'} - \boldsymbol{r}_{fn})} \int_{S_n} d\boldsymbol{r}' e^{-i\boldsymbol{k}\cdot(\boldsymbol{r}' - \boldsymbol{r}_{fn})} \boldsymbol{b}_n(\boldsymbol{r}').$$

Fast Multipole Method

Evaluate the interactions in group-by-group manner:

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



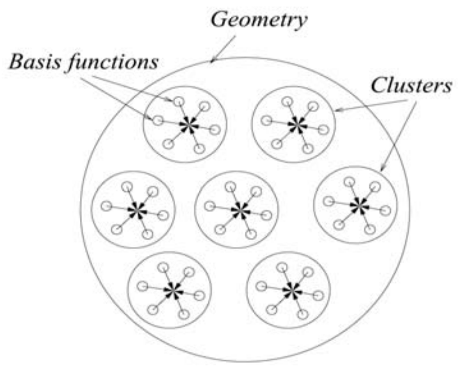
$$\boxed{Z_{mn}^{M} = \frac{k}{4\pi i} \int d^2\hat{\boldsymbol{k}} \boldsymbol{F}_{fmc}^{M}(\hat{\boldsymbol{k}}) T_L(k, |\boldsymbol{r}_{cc'}|, \hat{\boldsymbol{r}}_{cc'} \cdot \hat{\boldsymbol{k}}) \cdot \boldsymbol{F}_{fnc'}^{M}(\hat{\boldsymbol{k}})}$$

$$\boldsymbol{F}_{fmc}^{M}(\hat{\boldsymbol{k}}) = -\hat{\boldsymbol{k}} \times e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_{fm}-\boldsymbol{r}_c)} \int_{S_m} d\boldsymbol{r} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}_{fm})} \boldsymbol{t}_m(r) \times \hat{\boldsymbol{n}}$$

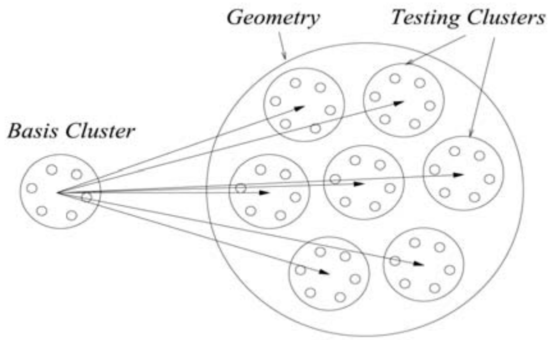
$$\boldsymbol{F}_{fnc'}^{M}(\hat{\boldsymbol{k}}) = e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_{c'}-\boldsymbol{r}_{fn})} \int_{S_n} d\boldsymbol{r}' e^{-i\boldsymbol{k}\cdot(\boldsymbol{r}'-\boldsymbol{r}_{fn})} \boldsymbol{b}_n(\boldsymbol{r}').$$

Computational Electromagnetics Laboratory

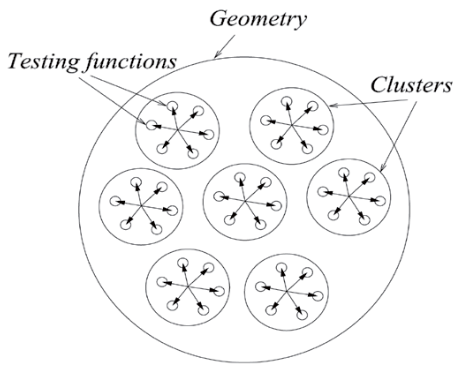
Fast Multipole Method (Steps)



Aggregation



Translation

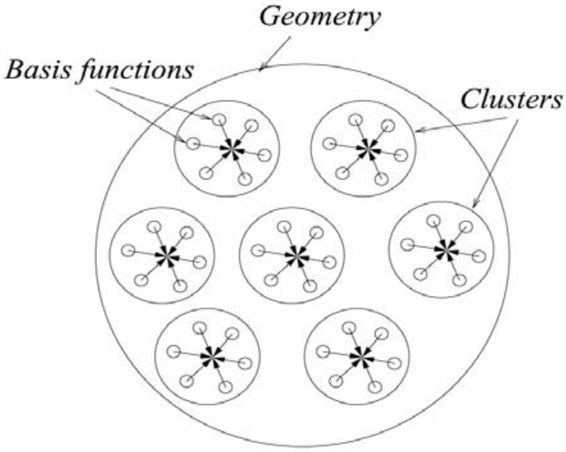


Disaggregation

Fast Multipole Method (FMM)

- Three steps of FMM:

(1) Aggregation:



Radiation of group C′

Radiation of the basis function

$$\boxed{\boldsymbol{F}^{C'}(\hat{\boldsymbol{k}})} = \sum_{n\in C'} \boxed{\boldsymbol{F}^{M}_{fnc'}(\hat{\boldsymbol{k}})}\, a_n$$

$$\boxed{\boldsymbol{F}^{C'}(\hat{\boldsymbol{k}}) = \int_{S_n} d\boldsymbol{r}' \exp(-ik\cdot(\boldsymbol{r}' - \boldsymbol{r}_{C'}))(\bar{\boldsymbol{I}} - \hat{\boldsymbol{k}}\hat{\boldsymbol{k}})\cdot \boldsymbol{b}_n(\boldsymbol{r}')}$$

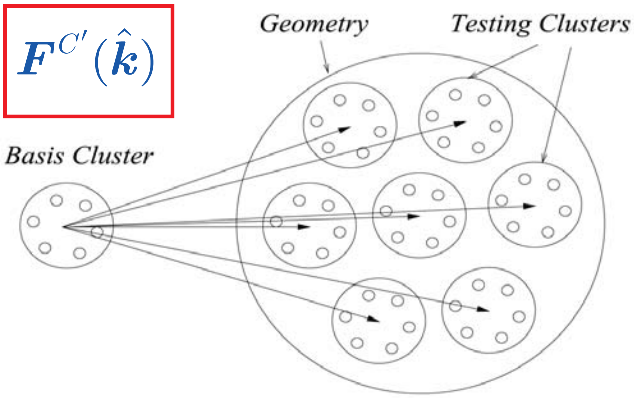
Fast Multipole Method (FMM)

(2) Translation:

Radiation of group C′

$$\boxed{\boldsymbol{F}^{C}_{T}(\hat{\boldsymbol{k}})} = \sum_{C'\notin N(C)} T_L(k, |\boldsymbol{r}_{cc'}|, \hat{\boldsymbol{r}}_{cc'}\cdot\hat{\boldsymbol{k}})\, \boxed{\boldsymbol{F}^{C'}(\hat{\boldsymbol{k}})}$$

Incoming wave for group C



Translation function

$$T_L(k, |\boldsymbol{r}_{cc'}|, \hat{\boldsymbol{r}}_{cc'}\cdot\hat{\boldsymbol{k}}) = \frac{ik}{4\pi}\sum_{l=0}^{L} i^l(2l+1)h_l^{(1)}(k\,|\boldsymbol{r}_{cc'}|)P_l\left(\hat{\boldsymbol{r}}_{cc'}\cdot\hat{\boldsymbol{k}}\right)$$

Error Source: Truncation of an infinite summation

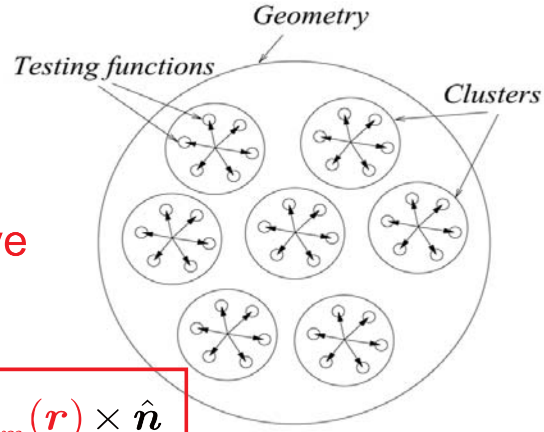
Fast Multipole Method (FMM)

(3) Disaggregation and reception:

$$\sum_{n=1}^{N} Z_{mn} a_n = \frac{1}{4\pi}\int d^2\hat{\boldsymbol{k}}\, \boxed{\boldsymbol{F}_{fmc}(\hat{\boldsymbol{k}})} \cdot \boxed{\boldsymbol{F}_T^C(\hat{\boldsymbol{k}})}$$

Receiving pattern of the testing function

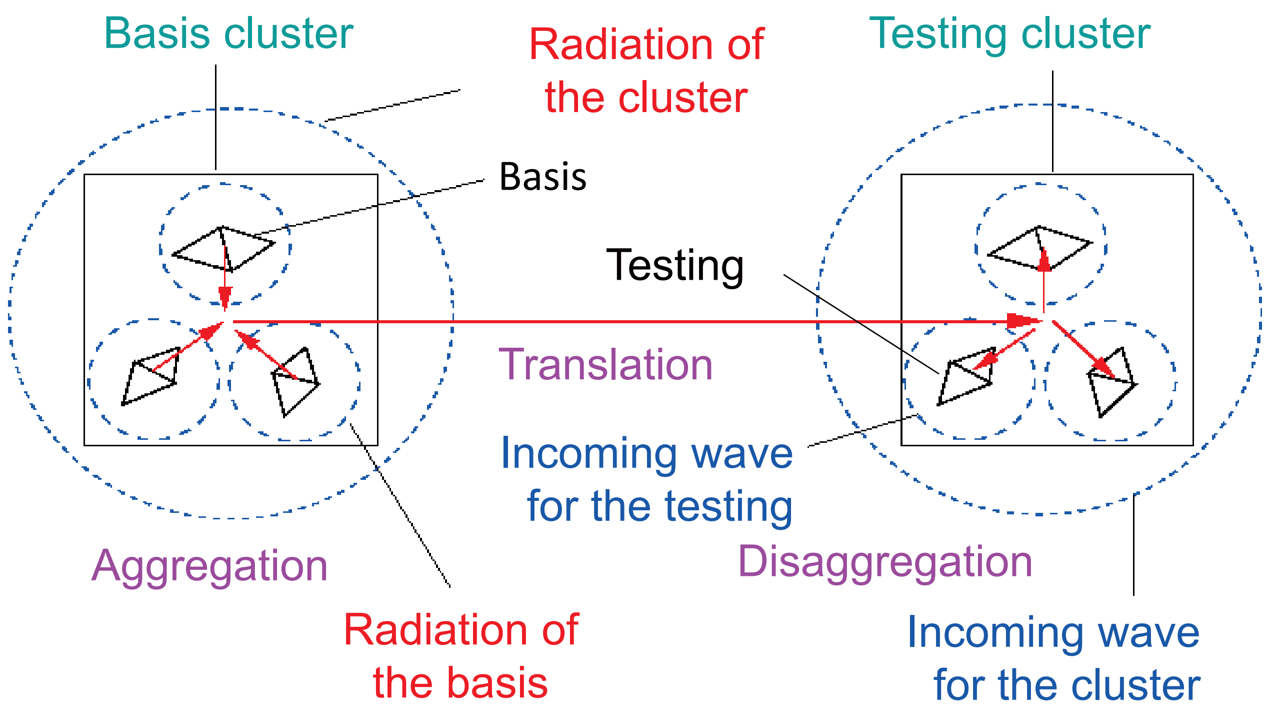
Incoming wave for group C



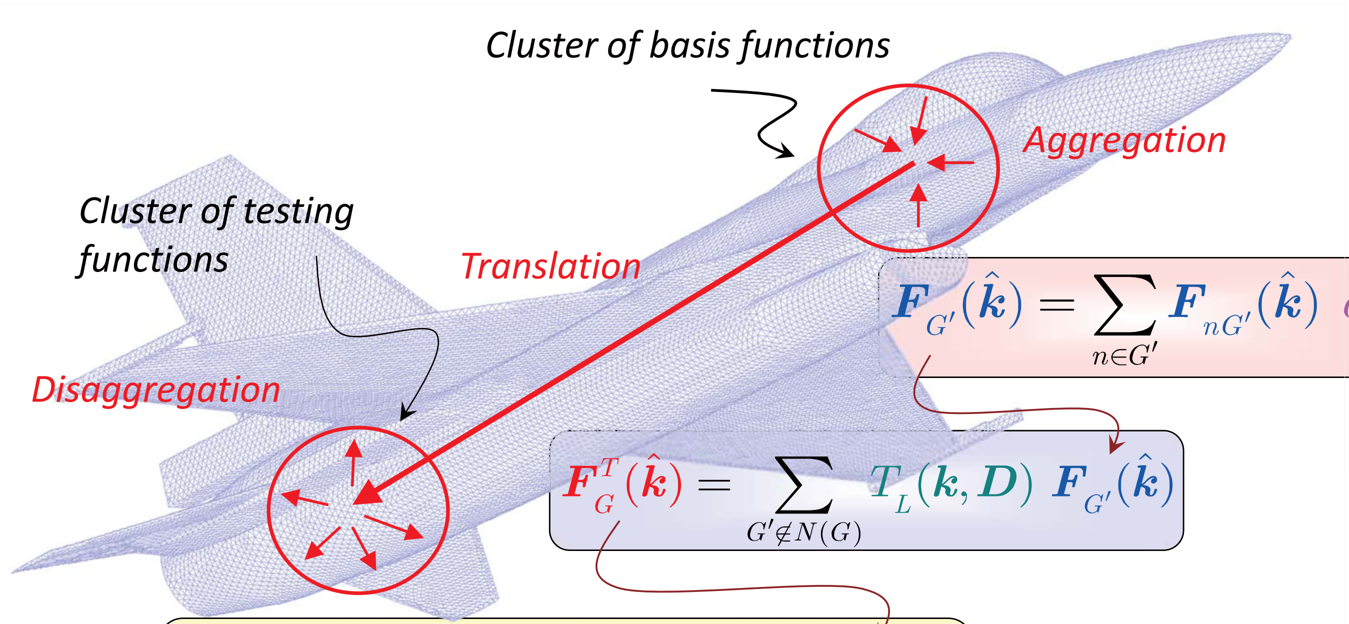
$$\boxed{\boldsymbol{F}^M_{fmc}(\hat{\boldsymbol{k}}) = -\hat{\boldsymbol{k}} \times \int_{S_m} d\boldsymbol{r} \exp(i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}_c))\boldsymbol{t}_m(\boldsymbol{r}) \times \hat{\boldsymbol{n}}}$$

Error Source: Angular integration over unit sphere

Fast Multipole Method (FMM)



Fast Multipole Method



$$\boldsymbol{F}_{G'}(\hat{\boldsymbol{k}}) = \sum_{n\in G'} \boldsymbol{F}_{nG'}(\hat{\boldsymbol{k}})\; a_n$$

$$\boldsymbol{F}^T_G(\hat{\boldsymbol{k}}) = \sum_{G'\notin N(G)} T_L(\boldsymbol{k},\boldsymbol{D})\; \boldsymbol{F}_{G'}(\hat{\boldsymbol{k}})$$

$$\sum_{n=1}^{N} Z_{mn} a_n = \frac{1}{4\pi}\int d^2\hat{\boldsymbol{k}}\; \boldsymbol{F}^C_{mG}(\hat{\boldsymbol{k}})\cdot \boldsymbol{F}^T_G(\hat{\boldsymbol{k}})$$

Fast Multipole Method (FMM)

$$\sum_{n=1}^{N} Z_{mn} a_n = \boxed{\sum_{C'\in N(C)} \sum_{n\in C'} Z_{mn} a_n}$$

Near-field interactions

$$+\frac{1}{4\pi}\int d^2\hat{\boldsymbol{k}}\boldsymbol{F}_{fmc}(\hat{\boldsymbol{k}})\cdot \sum_{C'\notin N(C)} T_L(k,\left|\boldsymbol{r}_{cc'}\right|,\hat{\boldsymbol{r}}_{cc'}\cdot\hat{\boldsymbol{k}}) \sum_{n\in C'} \boldsymbol{F}_{fnc'}(\hat{\boldsymbol{k}}) a_n$$

Far-field interactions

$$m = 1, 2, \ldots N$$

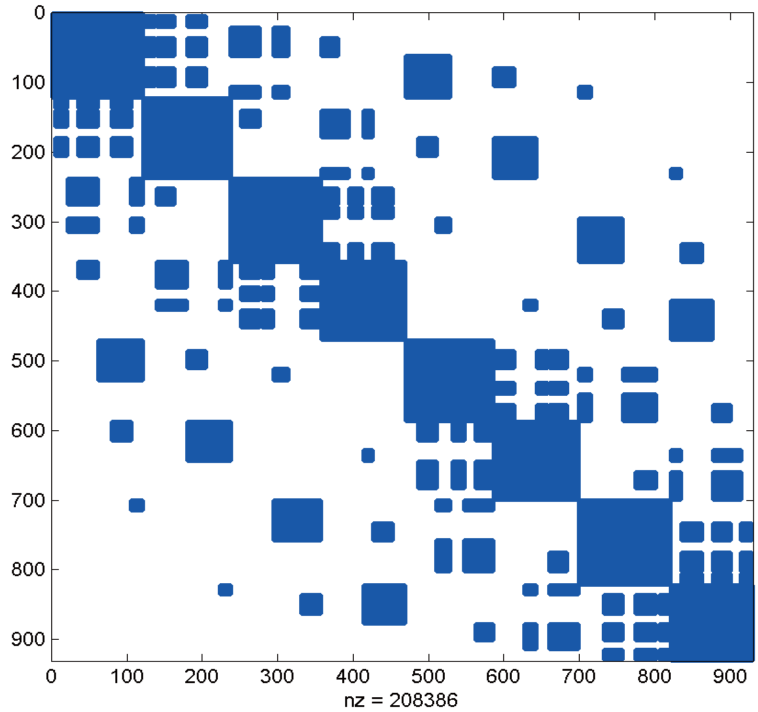
1) FMM performs matrix-vector multiplications (required by the iterative solver) with $O(N^{3/2})$ FLOPs.

2) Only the near-field interactions are stored in the memory so that the memory requirement is also reduced to $O(N^{3/2})$.

3) Hence, we are able to solve larger problems with the FMM.

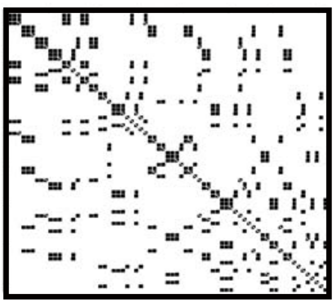
Near-Field Matrix

930
unknowns

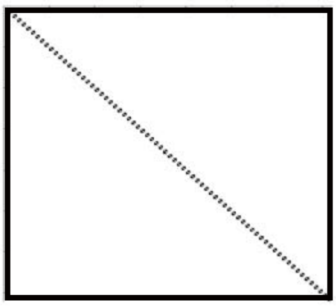


Sparsity
%24

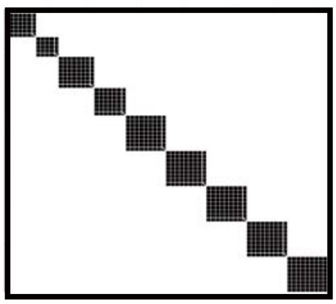
Preconditioners



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



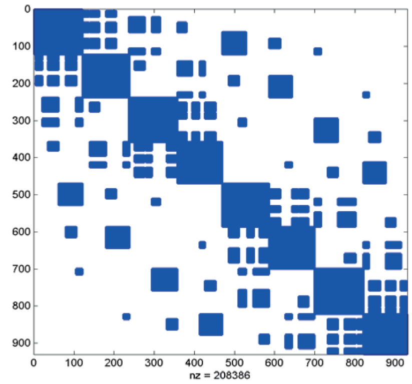
Diagonal:
- Diagonal (self-unknown) elements in the impedance matrix are selected
- Size is fixed
- Easy to factorize and use



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

Preconditioners

Sparse Near-Field Matrix:



- LU
- ILU: Incomplete LU
- SAI: Sparse Approximate Inverse
- INF: Iterative Near Field Preconditioner
- Use more than the available near-field matrix?

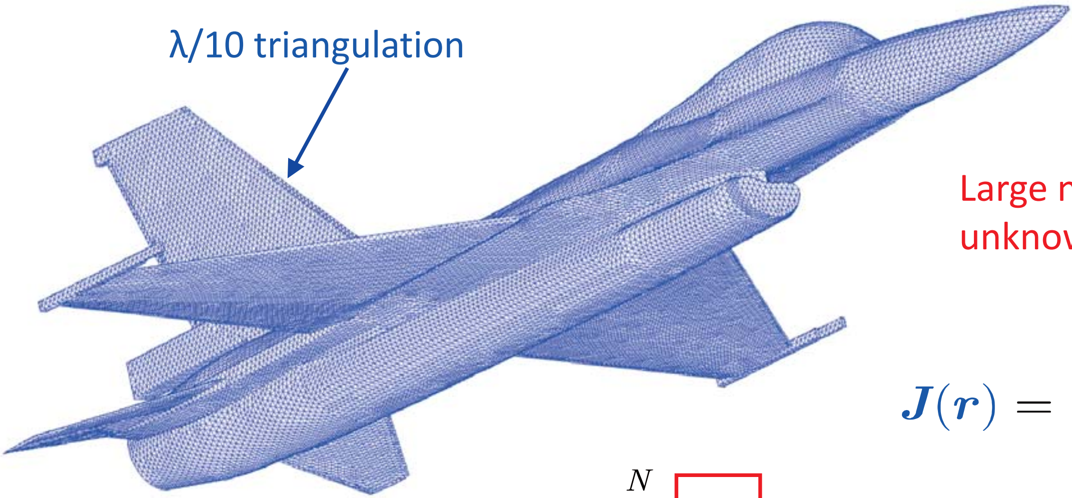
Multilevel Fast Multipole Algorithm (MLFMA)

Prof. Levent Gürel
CEO, ABAKUS Computing Technologies
Adjunct Professor, ECE, Univ. of Illinois at Urbana-Champaign

May 2015

ABAKÜS

Method of Moments



Large numbers of unknowns

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

- Matrix-equations: (Dense and Large)

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

Example (PEC-EFIE):

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

Solutions of Matrix-Equations

- Solve

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

- Iterative Solutions:

Matrix-Vector Multiplication

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

$\boldsymbol{x}$

$\boldsymbol{y}$

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

We need acceleration techniques.

MOM: Evaluating the Interactions

EFIE

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

MFIE

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

Integral Equations, Fast Algorithms, and Parallelization Strategies for the Solution of
Extremely Large Problems in Computational Electromagnetics - Part 1

Fast Multipole Method (FMM)

- Addition theorem (factorization of Green's function)

$$g(\boldsymbol{r},\boldsymbol{r}') = \frac{\exp\left(ik\left|\boldsymbol{D}+\boldsymbol{d}\right|\right)}{4\pi\left|\boldsymbol{D}+\boldsymbol{d}\right|} = \frac{ik}{4\pi}\sum_{l=0}^{\infty}(-1)^l(2l+1)j_l(kd)h_l^{(1)}(kD)P_l(\hat{\boldsymbol{d}}\cdot\hat{\boldsymbol{D}}) \qquad d \leq D$$

- Plane-wave expansion

$$4\pi i^l j_l(kd)P_l(\hat{\boldsymbol{d}}\cdot\hat{\boldsymbol{D}}) = \int d^2\hat{\boldsymbol{k}}\exp(ik\hat{\boldsymbol{k}}\cdot\boldsymbol{d})P_l(\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{D}})$$

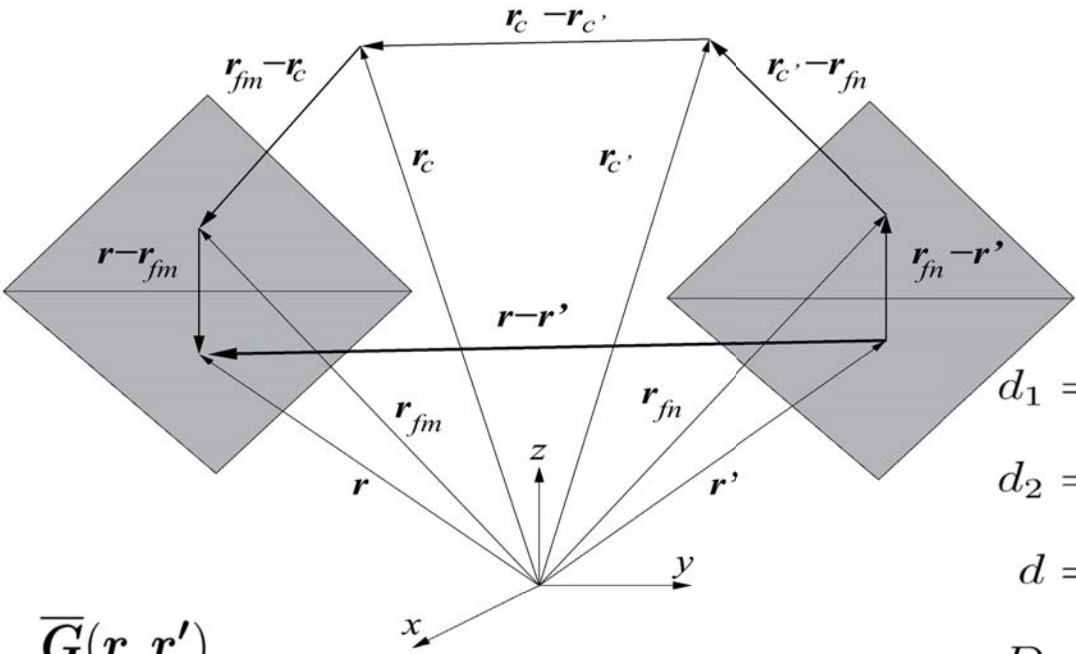
- Diagonalization

$$\frac{\exp\left(ik\left|\boldsymbol{D}+\boldsymbol{d}\right|\right)}{4\pi\left|\boldsymbol{D}+\boldsymbol{d}\right|} \approx \frac{1}{4\pi}\int d^2\hat{\boldsymbol{k}}\exp(ik\hat{\boldsymbol{k}}\cdot\boldsymbol{d})T_L(k,\hat{\boldsymbol{k}},\boldsymbol{D})$$

- Translation function

$$T_L(k,\hat{\boldsymbol{k}},\boldsymbol{D}) = \frac{ik}{4\pi}\sum_{l=0}^{L} i^l(2l+1)h_l^{(1)}(kD)P_l(\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{D}})$$

FMM: Evaluating the Interactions



$$d_1 = \boldsymbol{r}_{rfm} + \boldsymbol{r}_{fmc}$$

$$d_2 = \boldsymbol{r}_{c'fn} + \boldsymbol{r}_{fnr'}$$

$$d = d_1 + d_2$$

$$D = \boldsymbol{r}_{cc'}$$

$$\overline{\boldsymbol{G}}(\boldsymbol{r},\boldsymbol{r}') \approx \frac{1}{4\pi}\int d^2\hat{\boldsymbol{k}}(\overline{\boldsymbol{I}} - \hat{\boldsymbol{k}}\hat{\boldsymbol{k}})e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_{rfm}+\boldsymbol{r}_{fmc}+\boldsymbol{r}_{c'fn}+\boldsymbol{r}_{fnr'})}T_L(k,|\boldsymbol{r}_{cc'}|,\hat{\boldsymbol{r}}_{cc'}\cdot\hat{\boldsymbol{k}})$$

FMM: Evaluating the Interactions

EFIE $$Z^E_{mn} = \frac{1}{4\pi}\int d^2\hat{\boldsymbol{k}}\boldsymbol{F}^E_{fmc}(\hat{\boldsymbol{k}})T_L(k,|\boldsymbol{r}_{cc'}|,\hat{\boldsymbol{r}}_{cc'}\cdot\hat{\boldsymbol{k}})\cdot\boldsymbol{F}^E_{fnc'}(\hat{\boldsymbol{k}})$$

MFIE $$Z^M_{mn} = \frac{k}{4\pi i}\int d^2\hat{\boldsymbol{k}}\boldsymbol{F}^M_{fmc}(\hat{\boldsymbol{k}})T_L(k,|\boldsymbol{r}_{cc'}|,\hat{\boldsymbol{r}}_{cc'}\cdot\hat{\boldsymbol{k}})\cdot\boldsymbol{F}^M_{fnc'}(\hat{\boldsymbol{k}})$$

EFIE $$\boldsymbol{F}^E_{fmc}(\hat{\boldsymbol{k}}) = e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_{fm}-\boldsymbol{r}_c)}\int_{S_m} d\boldsymbol{r}e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}_{fm})}(\overline{\boldsymbol{I}}-\hat{\boldsymbol{k}}\hat{\boldsymbol{k}})\cdot\boldsymbol{t}_m(r)$$

$$\boldsymbol{F}^E_{fnc'}(\hat{\boldsymbol{k}}) = e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_{c'}-\boldsymbol{r}_{fn})}\int_{S_n} d\boldsymbol{r}'e^{-i\boldsymbol{k}\cdot(\boldsymbol{r}'-\boldsymbol{r}_{fn})}(\overline{\boldsymbol{I}}-\hat{\boldsymbol{k}}\hat{\boldsymbol{k}})\cdot\boldsymbol{b}_n(\boldsymbol{r}')$$

MFIE $$\boldsymbol{F}^M_{fmc}(\hat{\boldsymbol{k}}) = -\hat{\boldsymbol{k}}\times e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_{fm}-\boldsymbol{r}_c)}\int_{S_m} d\boldsymbol{r}e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}_{fm})}\boldsymbol{t}_m(r)\times\hat{\boldsymbol{n}}$$

$$\boldsymbol{F}^M_{fnc'}(\hat{\boldsymbol{k}}) = e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_{c'}-\boldsymbol{r}_{fn})}\int_{S_n} d\boldsymbol{r}'e^{-i\boldsymbol{k}\cdot(\boldsymbol{r}'-\boldsymbol{r}_{fn})}\boldsymbol{b}_n(\boldsymbol{r}').$$

FMM Considerations

1) Truncation of infinite summation:

$$T_L(k, D, \theta) = \frac{ik}{4\pi} \sum_{l=0}^{L} i^l (2l+1) h_l^{(1)}(kD) P_l(cos\theta)$$

$$L \approx kd + 1.8 d_0^{2/3} (kd)^{1/3}$$

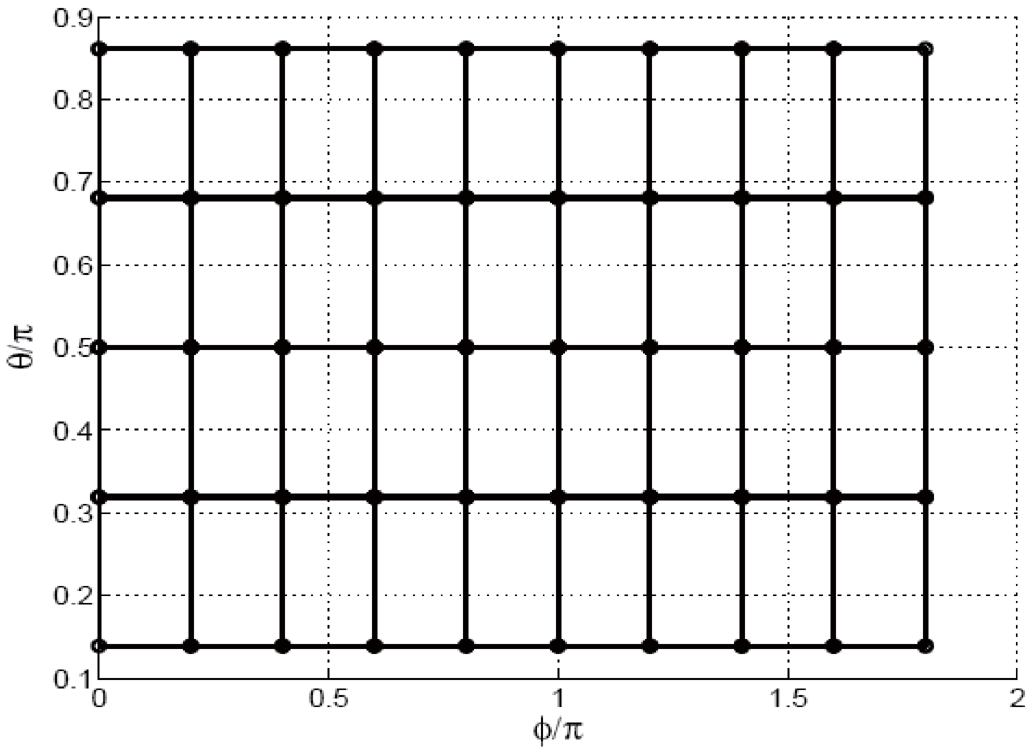
2) Angular integration:

$$Z_{mn}^M = \frac{k}{4\pi i} \int d^2\hat{\boldsymbol{k}} \boldsymbol{F}_{fmc}^M(\hat{\boldsymbol{k}}) T_L(k, |\boldsymbol{r}_{cc'}|, \hat{\boldsymbol{r}}_{cc'} \cdot \hat{\boldsymbol{k}}) \cdot \boldsymbol{F}_{fnc'}^M(\hat{\boldsymbol{k}})$$

$K=2L^2$

Angular Integration

Angular integration points for L = 5

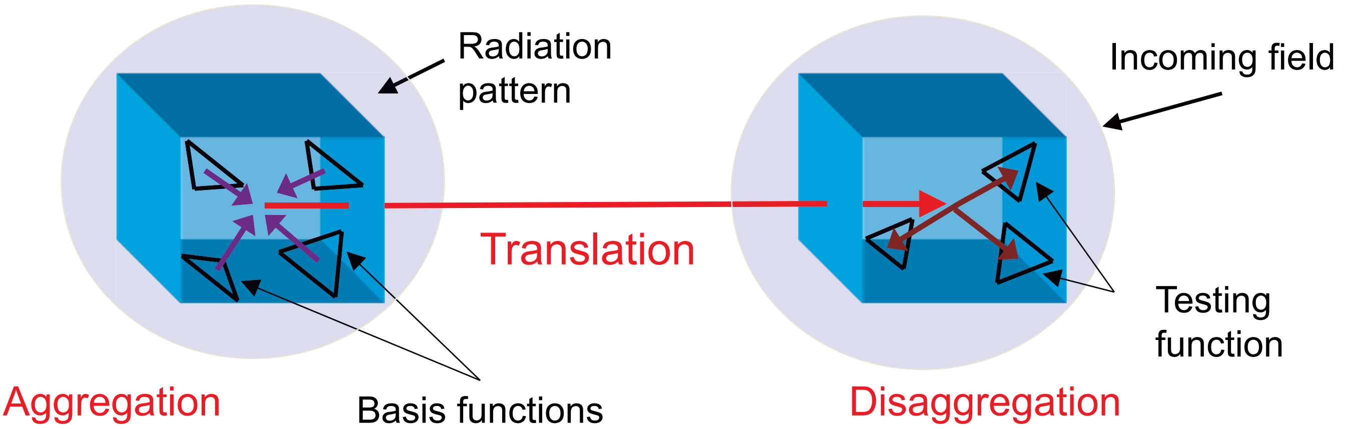


Fast Multipole Method

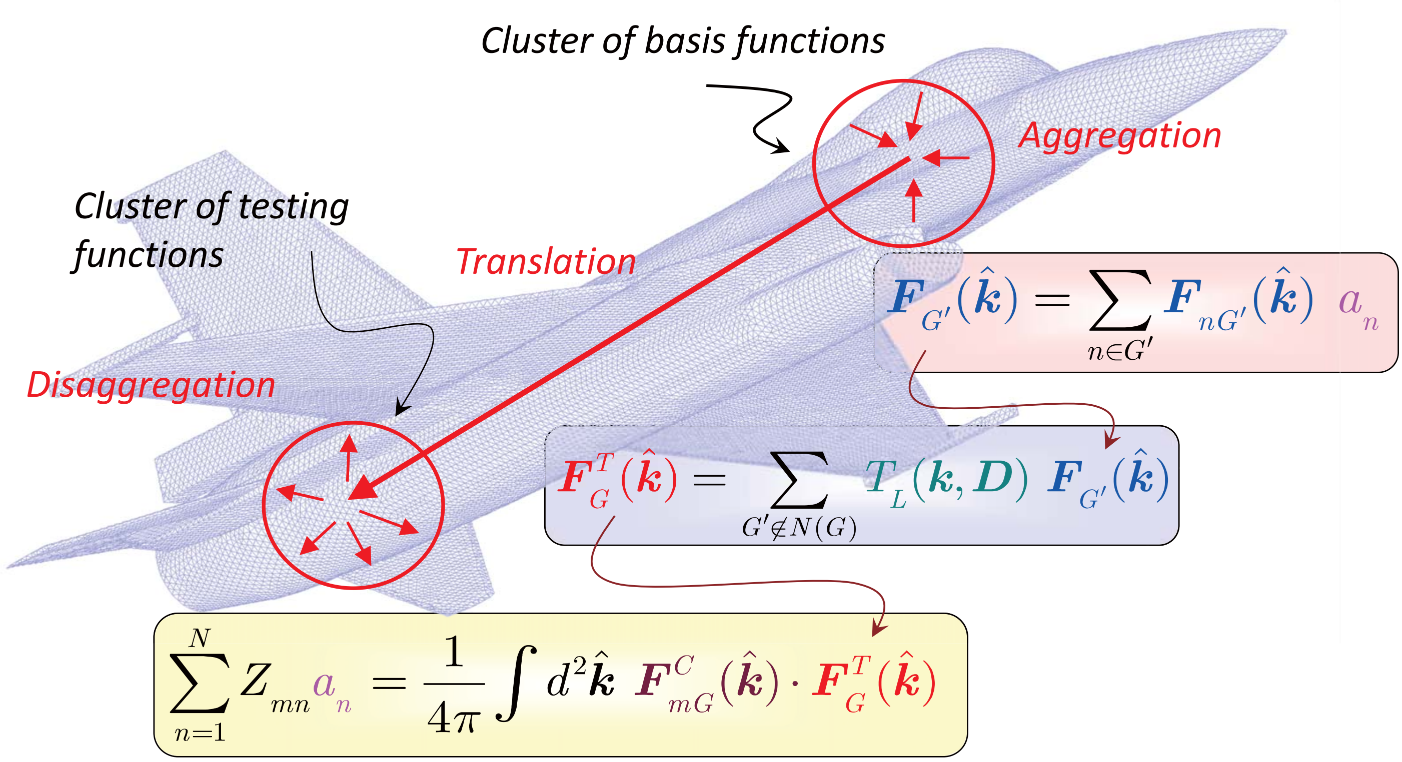
$$\sum_{n=1}^{N} Z_{mn} a_n = \boxed{\sum_{G' \in N(G)} \sum_{n \in G'} Z_{mn} a_n} \quad \text{Near-field interactions}$$

$$\boxed{+ \frac{1}{4\pi} \int d^2\hat{\boldsymbol{k}}\, \boldsymbol{F}_{mG}(\hat{\boldsymbol{k}}) \cdot \sum_{G' \notin N(G)} T_L(\boldsymbol{k}, \boldsymbol{r}_{GG'}) \sum_{n \in G'} \boldsymbol{F}_{nG'}(\hat{\boldsymbol{k}})\, a_n}$$

Far-field interactions $\qquad m = 1, 2, \ldots, N$



Fast Multipole Method

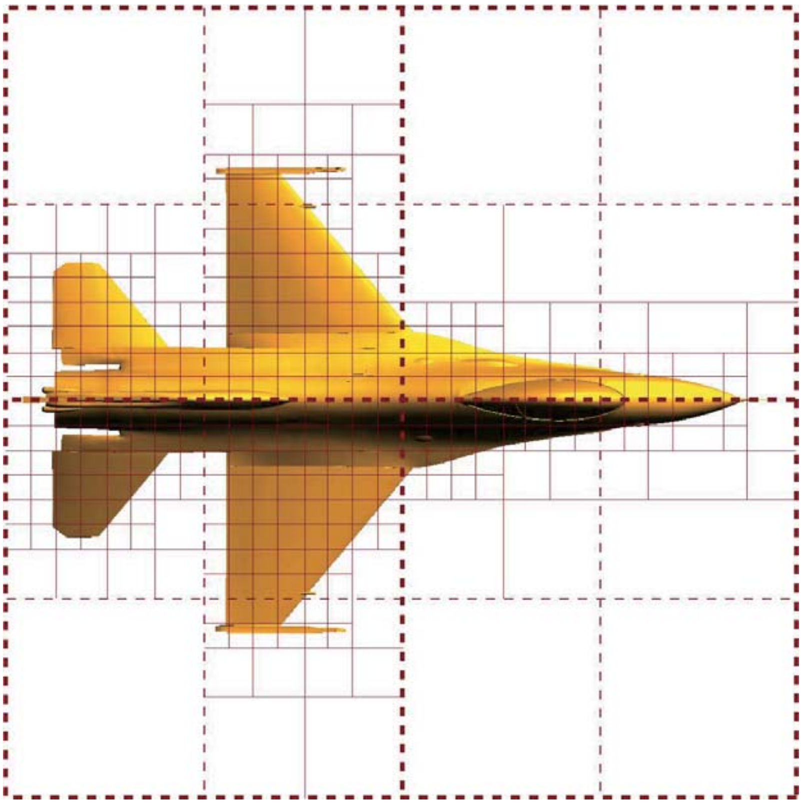


$$\boldsymbol{F}_{G'}(\hat{\boldsymbol{k}}) = \sum_{n \in G'} \boldsymbol{F}_{nG'}(\hat{\boldsymbol{k}})\; a_n$$

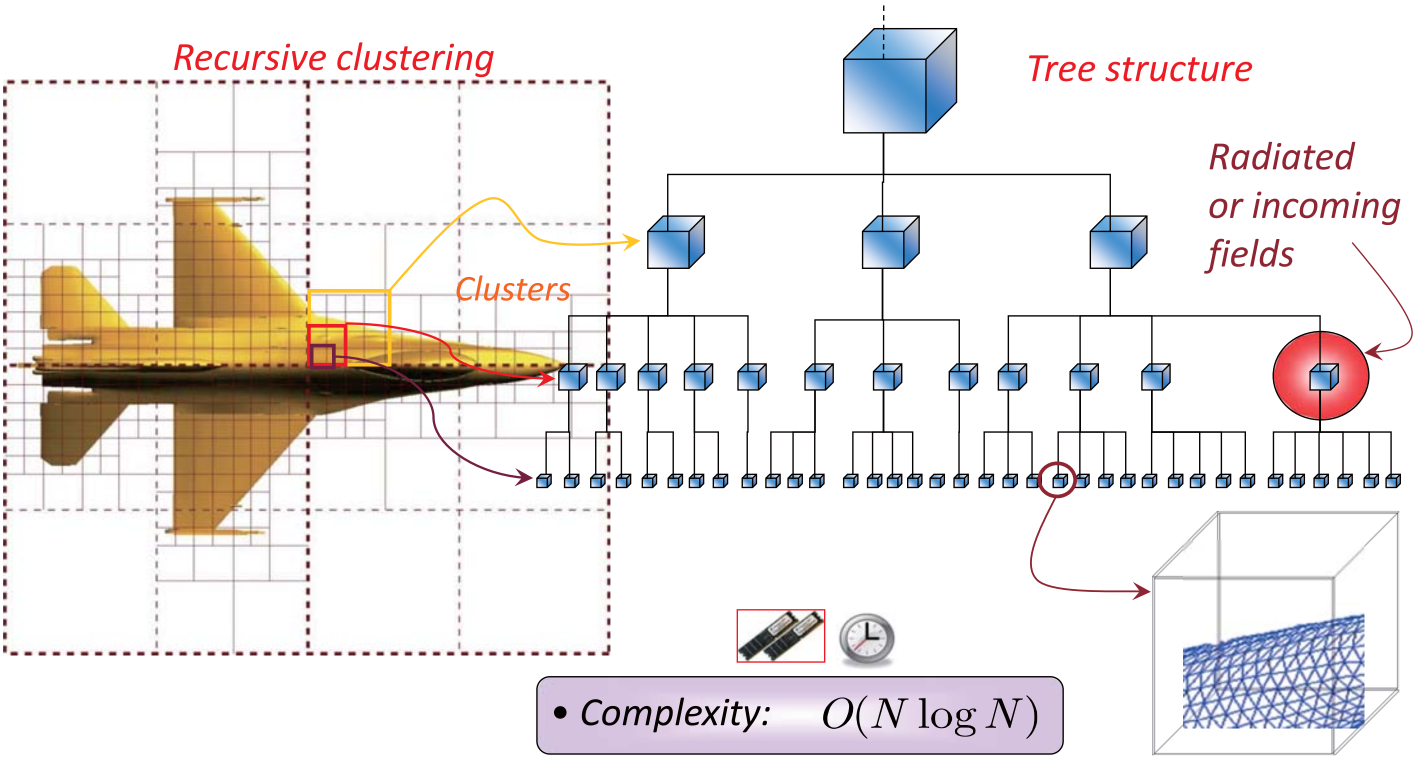
$$\boldsymbol{F}_G^T(\hat{\boldsymbol{k}}) = \sum_{G' \notin N(G)} T_L(\boldsymbol{k}, \boldsymbol{D})\; \boldsymbol{F}_{G'}(\hat{\boldsymbol{k}})$$

$$\sum_{n=1}^{N} Z_{mn} a_n = \frac{1}{4\pi} \int d^2\hat{\boldsymbol{k}}\; \boldsymbol{F}_{mG}^C(\hat{\boldsymbol{k}}) \cdot \boldsymbol{F}_G^T(\hat{\boldsymbol{k}})$$

Multilevel Fast Multipole Algorithm

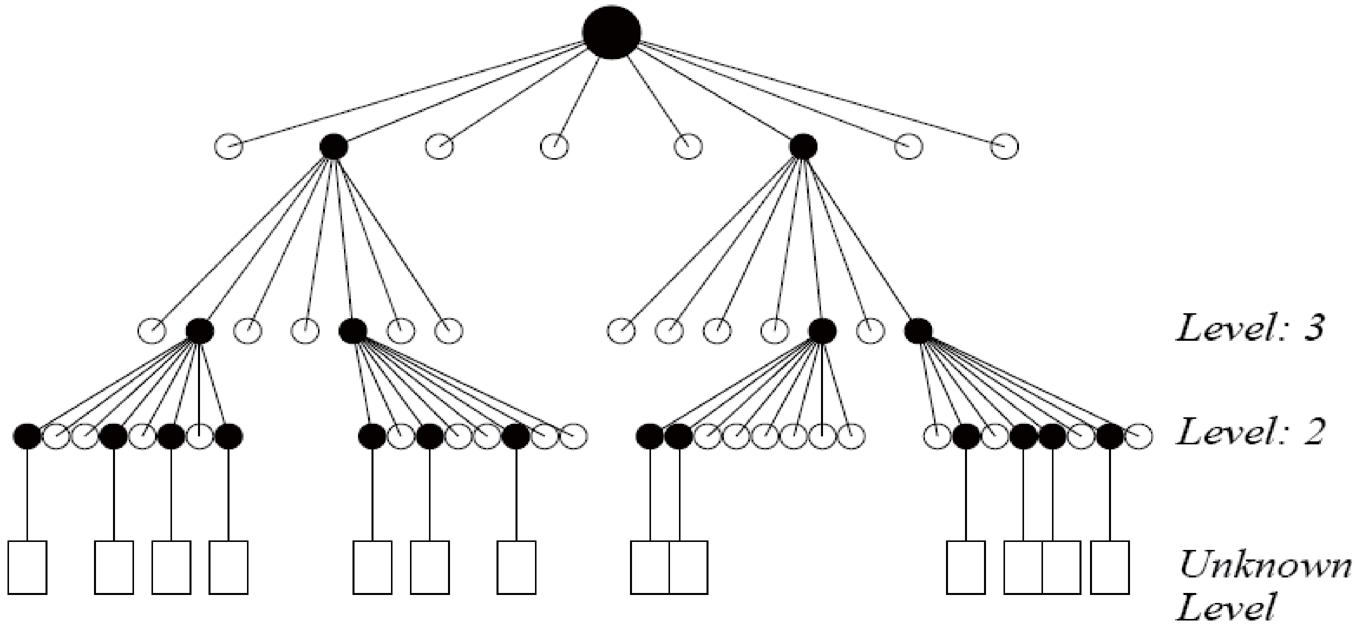


Multilevel Fast Multipole Algorithm

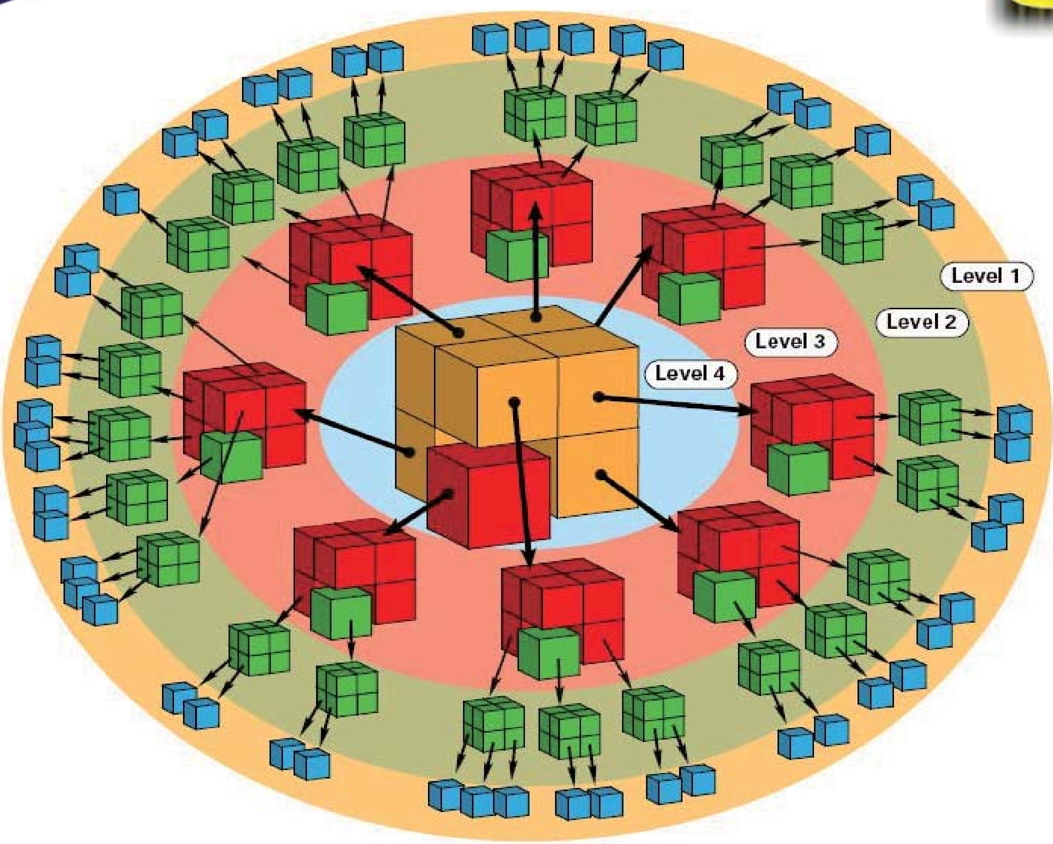


- *Complexity:* $O(N \log N)$

MLFMA Tree Structure

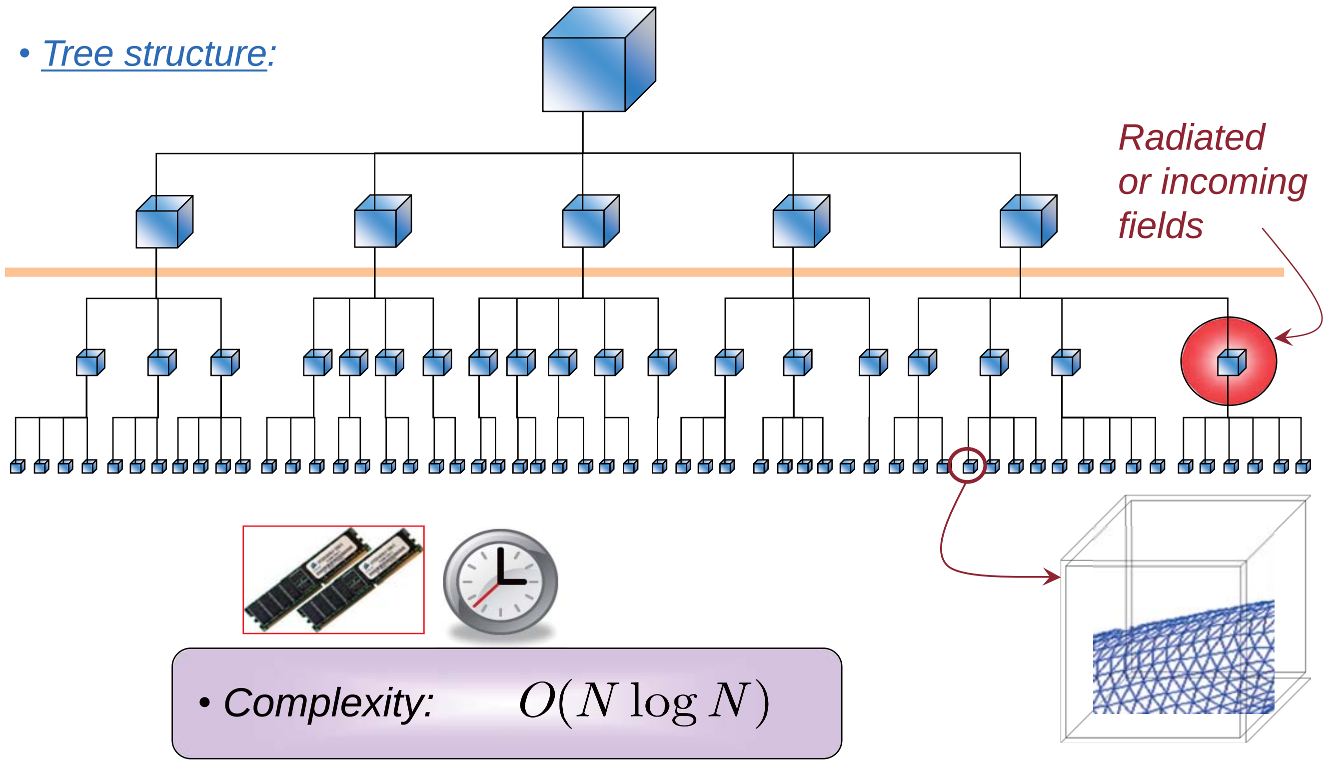


Recursive Clustering



Multilevel Fast Multipole Algorithm

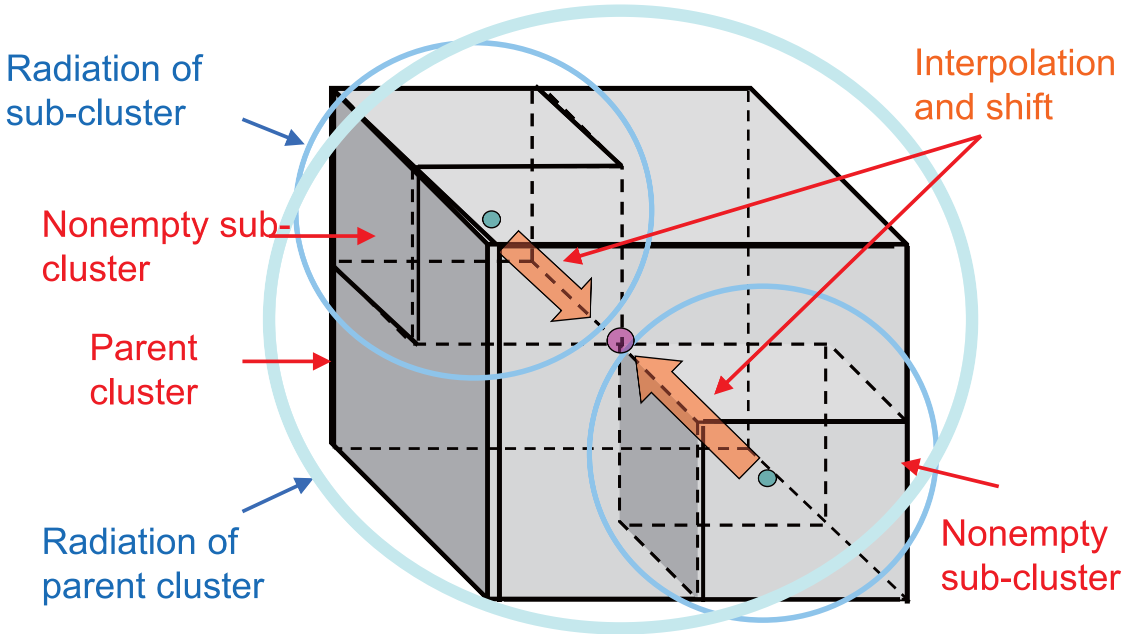
• *Tree structure:*



• *Complexity:* $O(N \log N)$

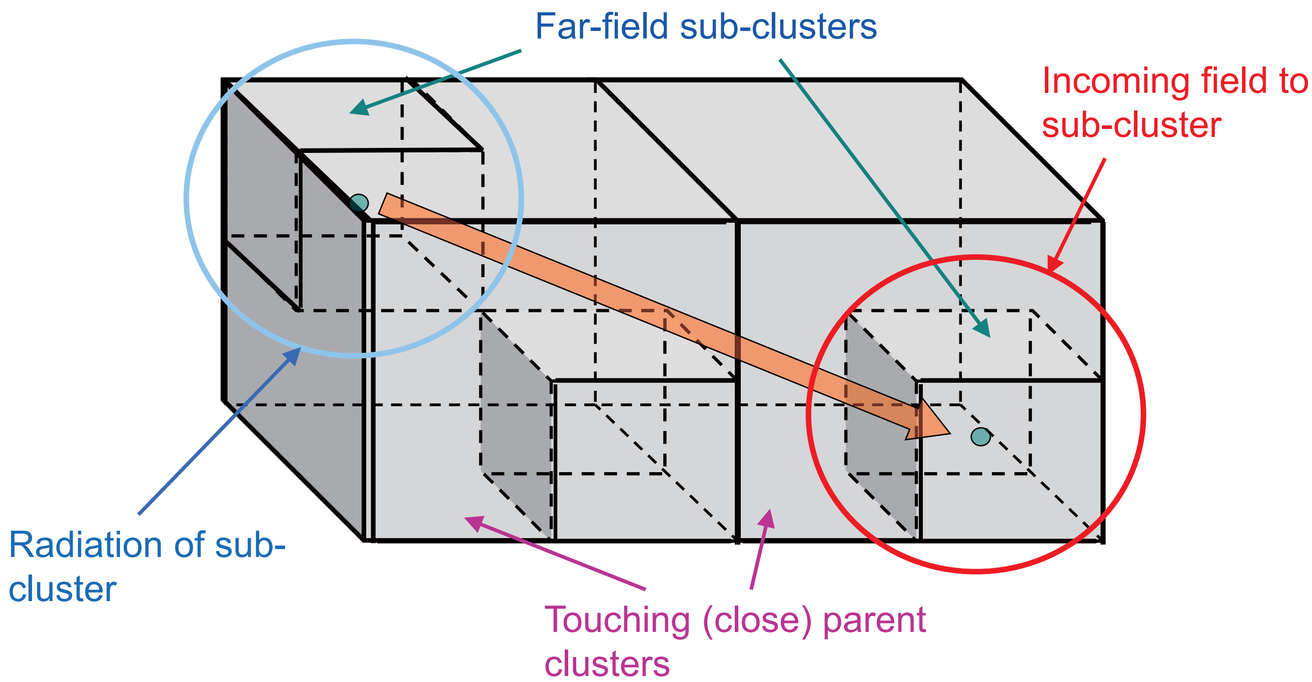
Multilevel Fast Multipole Algorithm

• Consider aggregation on the entire tree-structure.

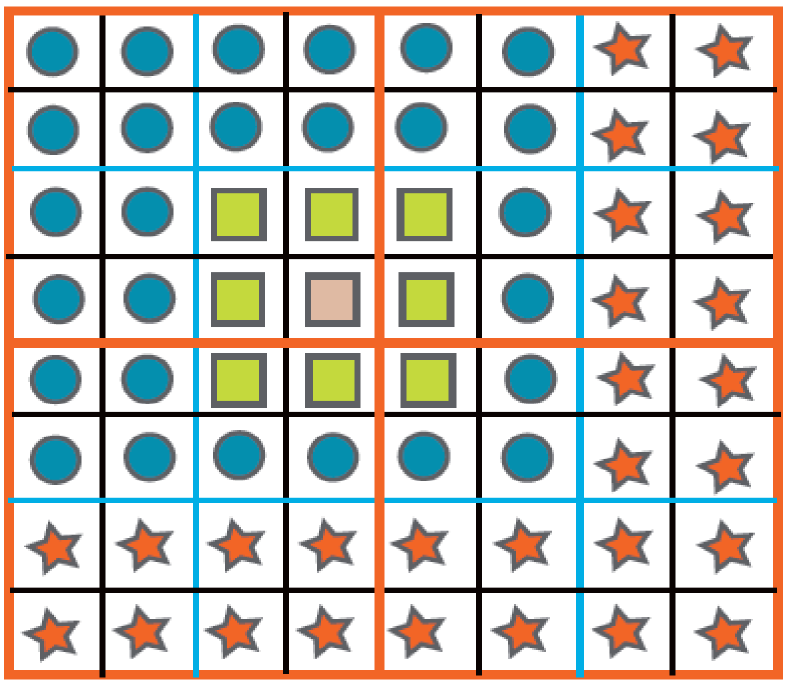


Multilevel Fast Multipole Algorithm

- Consider translation on the entire tree-structure.

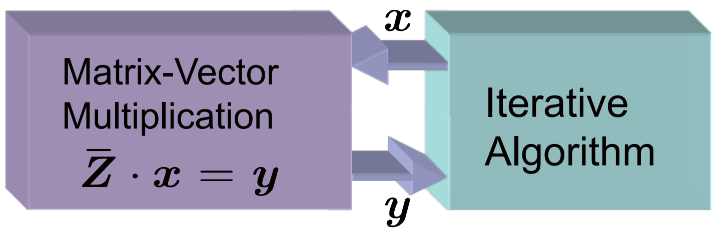


MLFMA Interactions



Acceleration with MLFMA

- Solve $\sum_{n=1}^{N} Z_{mn}^{E} a_n = v_m^E$



- Processing time for a matrix-vector product:

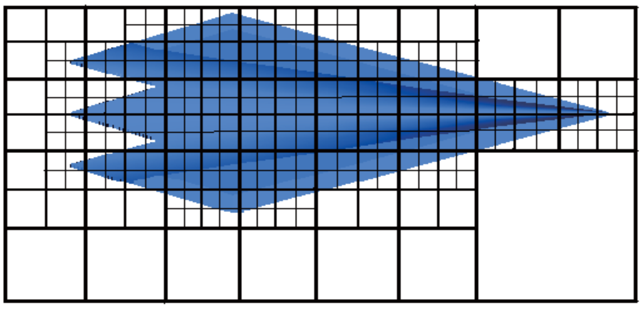
MOM [$O(N^2)$] → FMM [$O(N^{3/2})$] → MLFMA [$O(N\log N)$]

- Memory requirement:

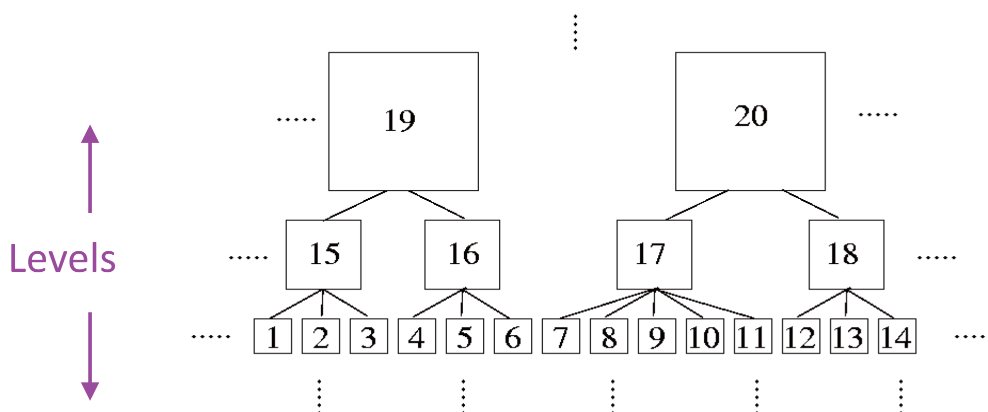
MOM [$O(N^2)$] → FMM [$O(N^{3/2})$] → MLFMA [$O(N\log N)$]

Multilevel FMM

- Apply the FMM concept in multi-level scheme:
  Group the groups!

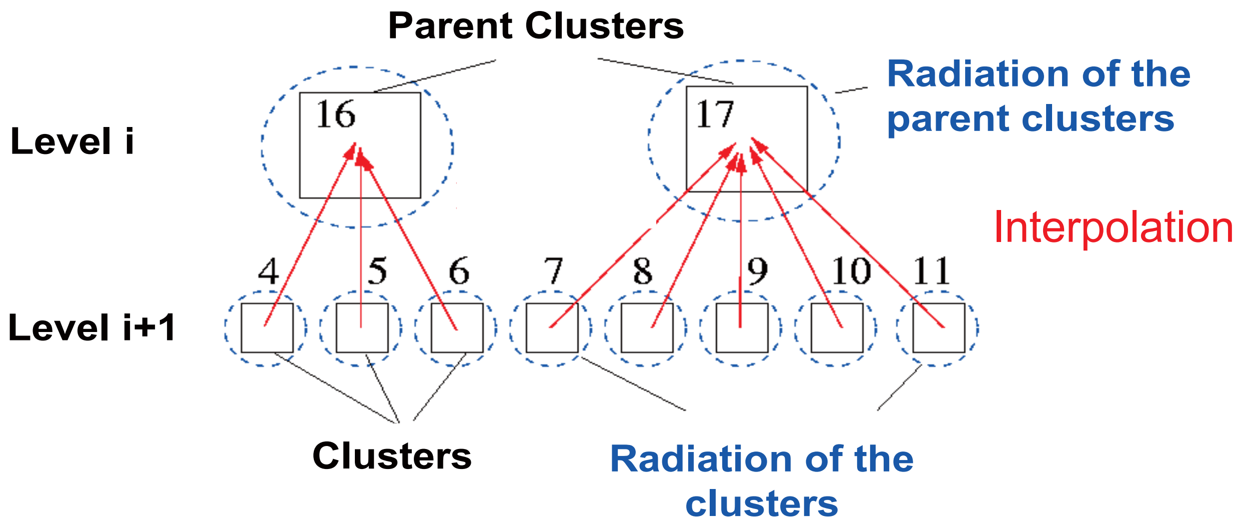


- Form tree structure:



Multilevel FMM

Aggregation between the levels



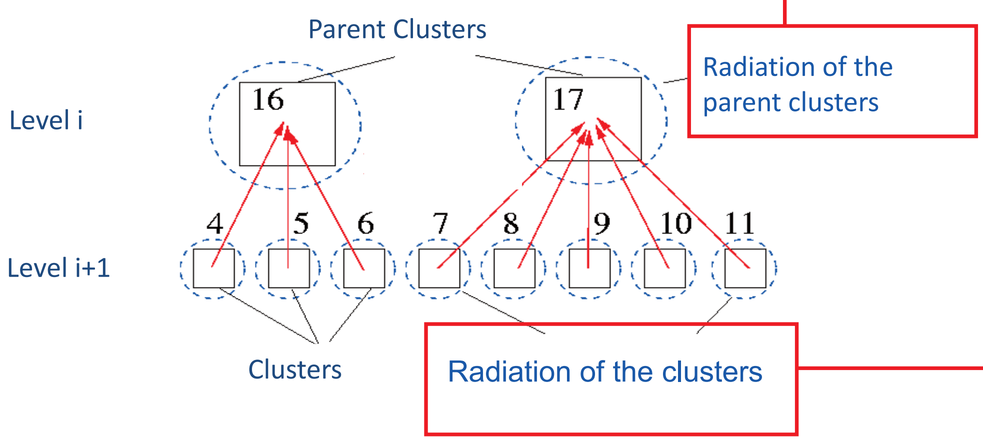
Multilevel FMM

Aggregation:

$$\boxed{\boldsymbol{F}^{C'_i}(\hat{\boldsymbol{k}})} = \sum_{C'_{i+1}\in G(C'_i)} \beta_{C'_i C'_{i+1}} \bar{\boldsymbol{I}}_{i,i+1} \cdot \boxed{\boldsymbol{F}^{C'_{i+1}}(\hat{\boldsymbol{k}})}$$

$$\beta_{C'_i C'_{i+1}} = \exp\left[i\boldsymbol{k}\cdot(\boldsymbol{r}_{C'_i} - \boldsymbol{r}_{C'_{i+1}})\right]$$

$\bar{\boldsymbol{I}}_{i,i+1}$: Interpolation

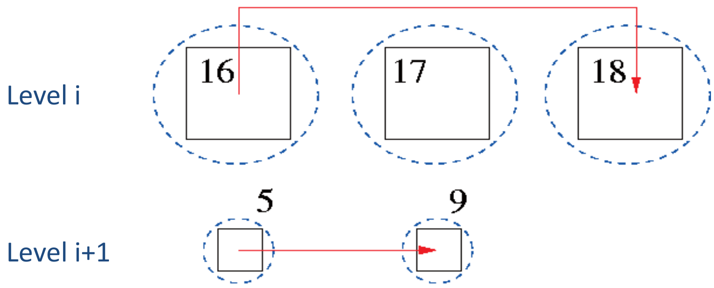


Multilevel FMM

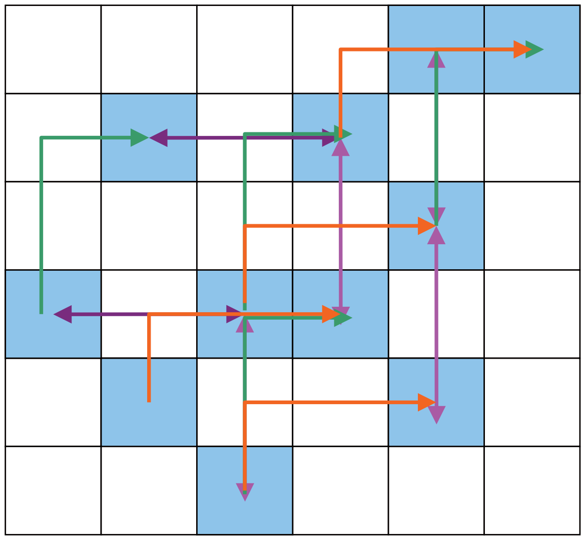
Translations: Required in each level.

$$\boldsymbol{F}_T^{C_i}(\hat{\boldsymbol{k}}) = \sum_{P(C_i')\in N(P(C_i))} \sum_{C_i'\in F(C_i)} T_L(k,|\boldsymbol{r}_{cc'}|, \hat{\boldsymbol{r}}_{cc'}\cdot\hat{\boldsymbol{k}})\ \boldsymbol{F}^{C_i'}(\hat{\boldsymbol{k}})$$

$$\tau(l) \approx 1.73ka_l + 2.16(d_0)^{2/3}(ka_l)^{1/3}$$

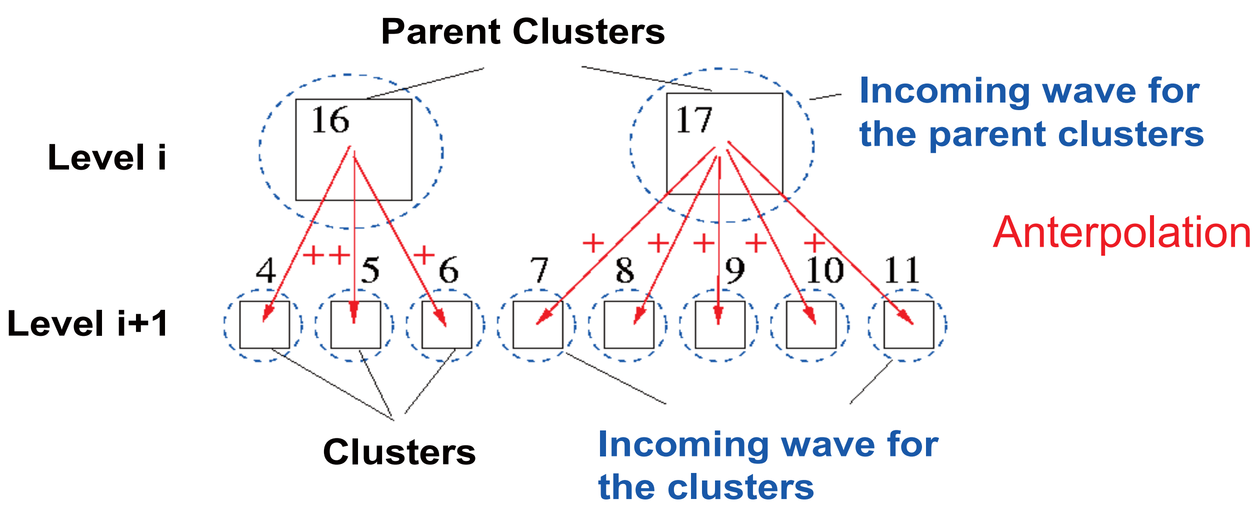


Use symmetry for efficiency:



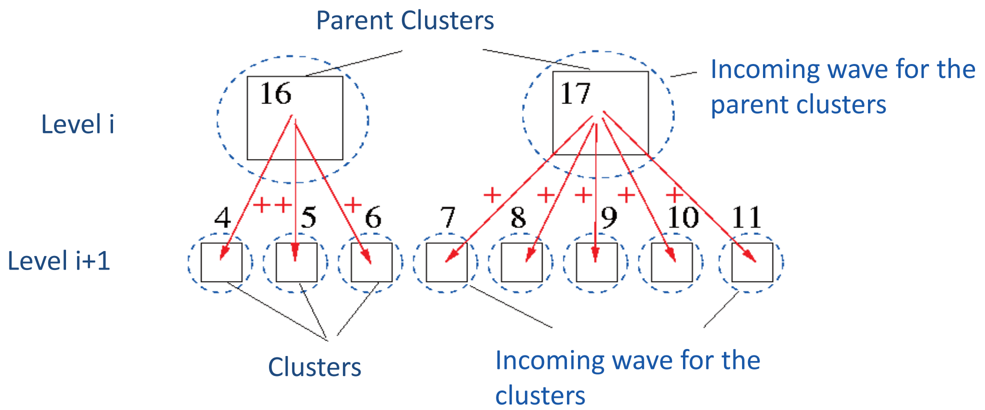
Multilevel FMM

Disaggregation between the levels



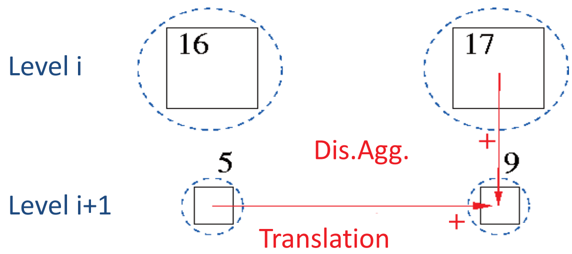
Multilevel FMM

Disaggregation:



Multilevel FMM

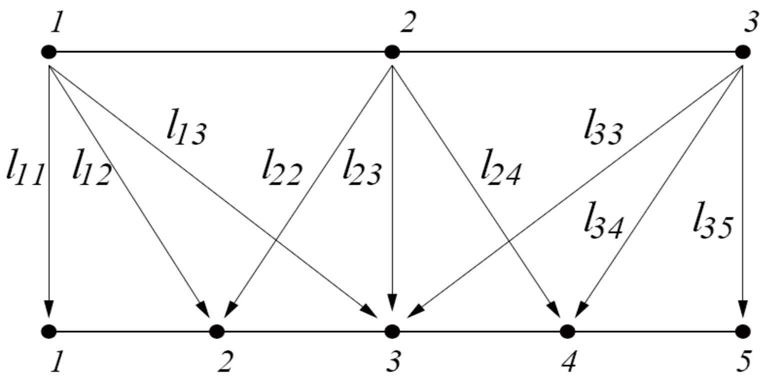
Disaggregation:

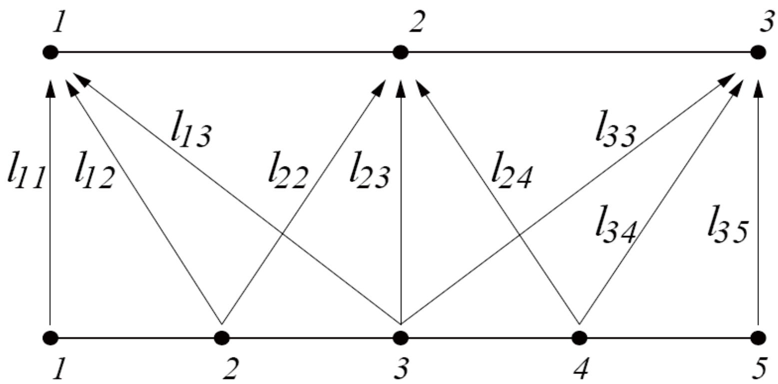


$$\boldsymbol{F}_{TD}^{C_{i+1}}(\hat{\boldsymbol{k}}) = \boxed{\boldsymbol{F}_{T}^{C_{i+1}}(\hat{\boldsymbol{k}})} + \overline{\boldsymbol{I}}_{i+1,i} \cdot \beta_{\boldsymbol{C}'_{i+1}\boldsymbol{C}'_i} \boxed{\boldsymbol{F}_{TD}^{P(C_{i+1})}(\hat{\boldsymbol{k}})}$$

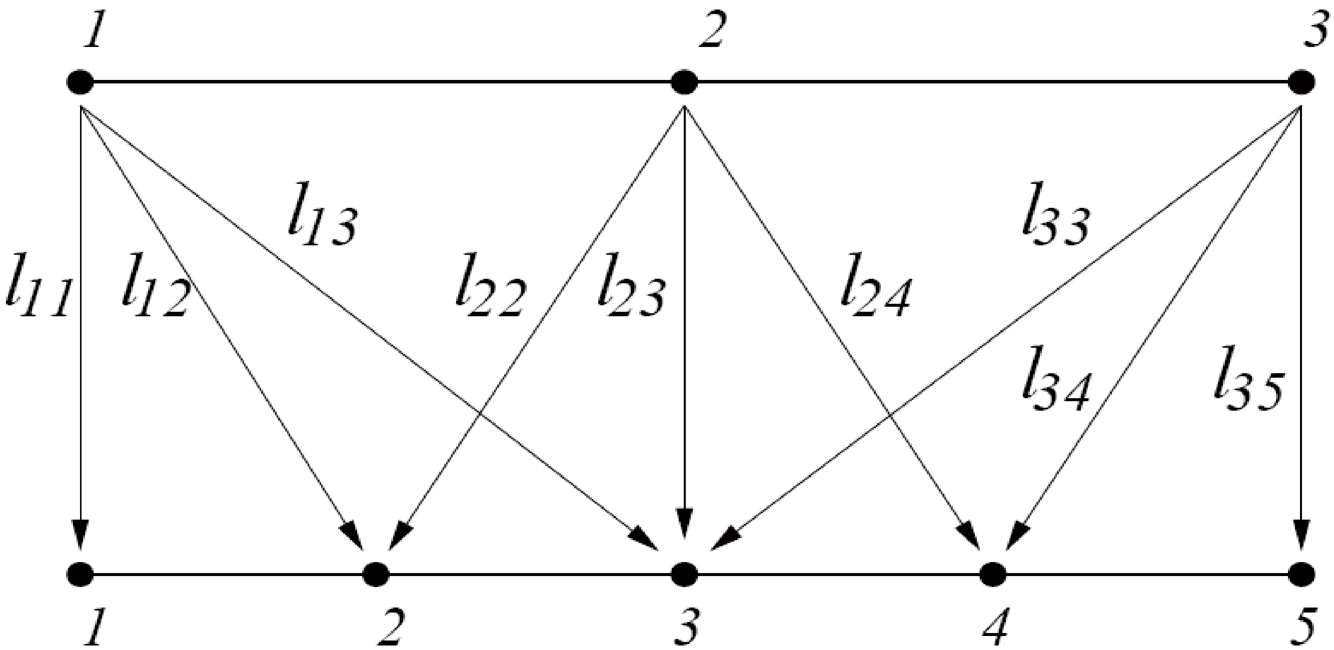
Translation Disaggregation

Interpolation and Anterpolation

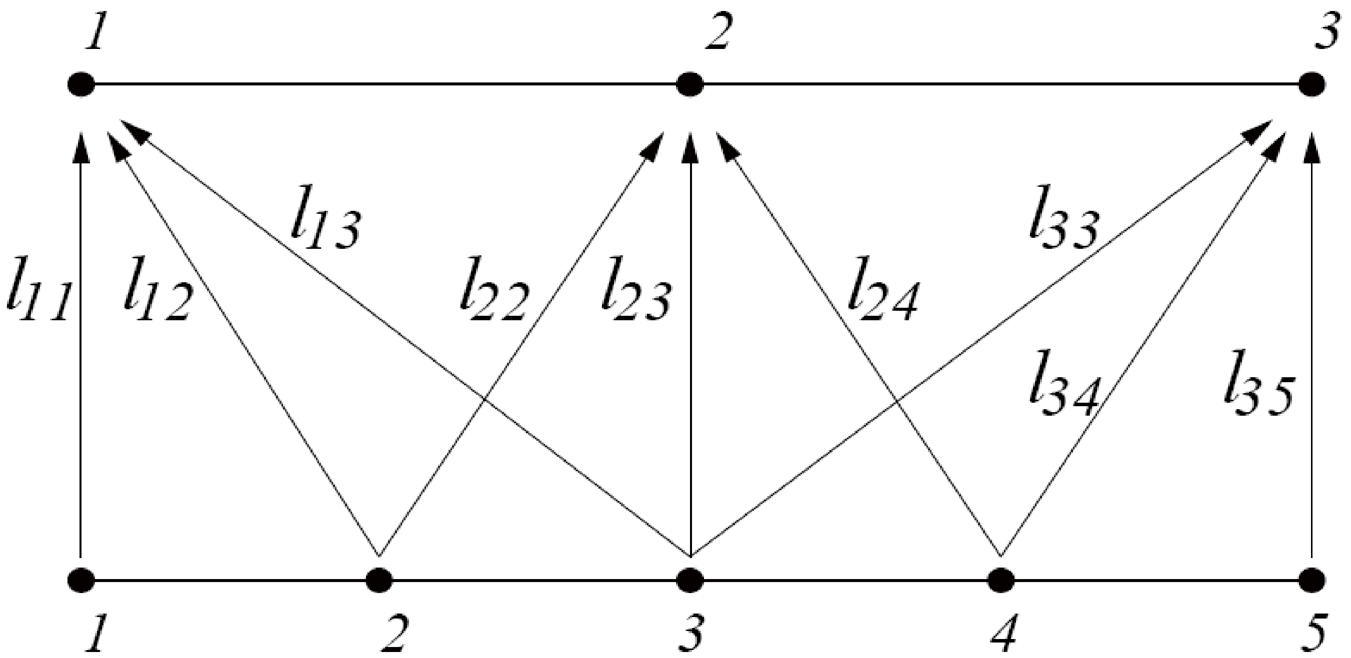




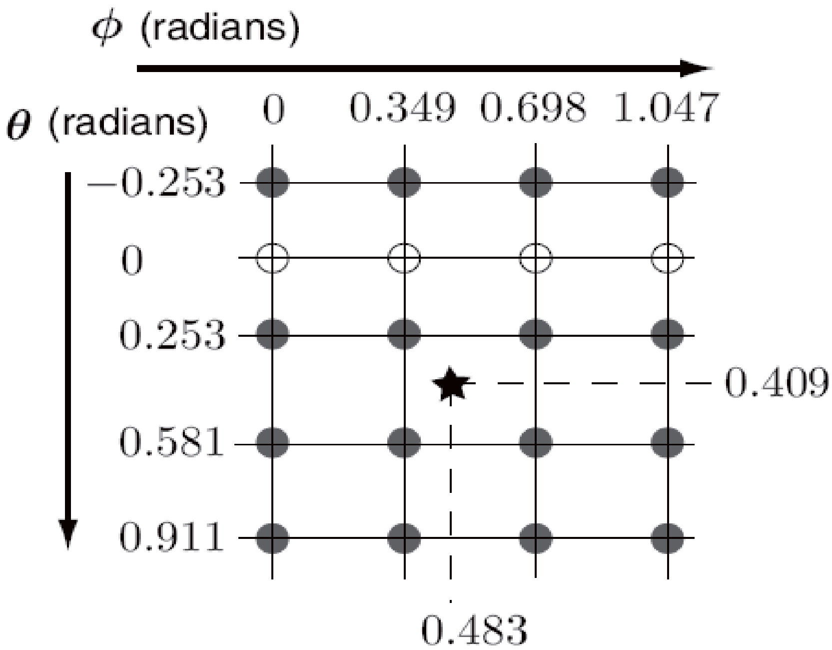
Interpolation



Anterpolation



Lagrange Interpolation



Lagrange interpolation employing 4×4 points (shaded circles) located in the coarse grid to evaluate the function at a point (star) located in the fine grid. Sampling values of ϑ and φ are specified in radians and selected from a practical case.

Multilevel FMM

- Between the levels
interpolation and anterpolation algorithms are required:

Error Source: Interpolation between levels

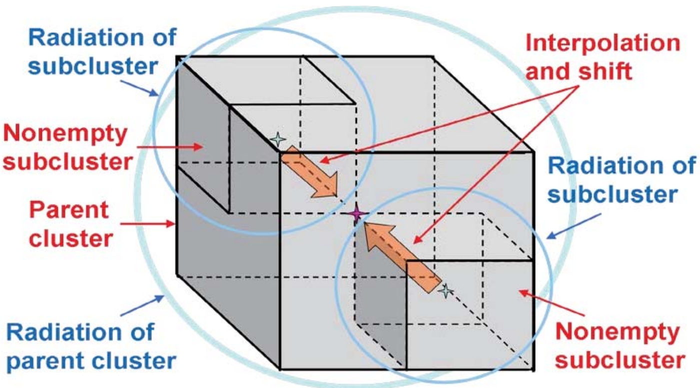
- Processing time for a matrix-vector product:

MOM [O(N^2)] → FMM [O(N$^{3/2}$)] → MLFMA [O(NlogN)]

- Memory requirement:

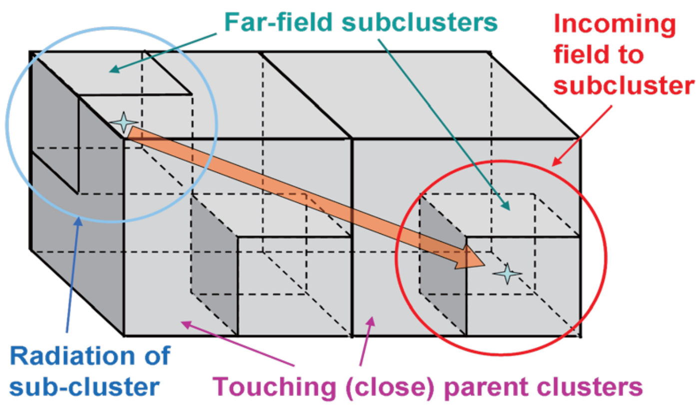
MOM [O(N^2)] → FMM [O(N$^{3/2}$)] → MLFMA [O(NlogN)]

Multilevel Fast Multipole Algorithm



Aggregation:
- Performed from bottom to top
- Local interpolations are used
- O(N) operations per level

Translation:
- O(1) testing clusters for each basis cluster
- O(N) operations per level
- O(1) different translation operators per level
(for cubic clusters)



Complexity of MLFMA

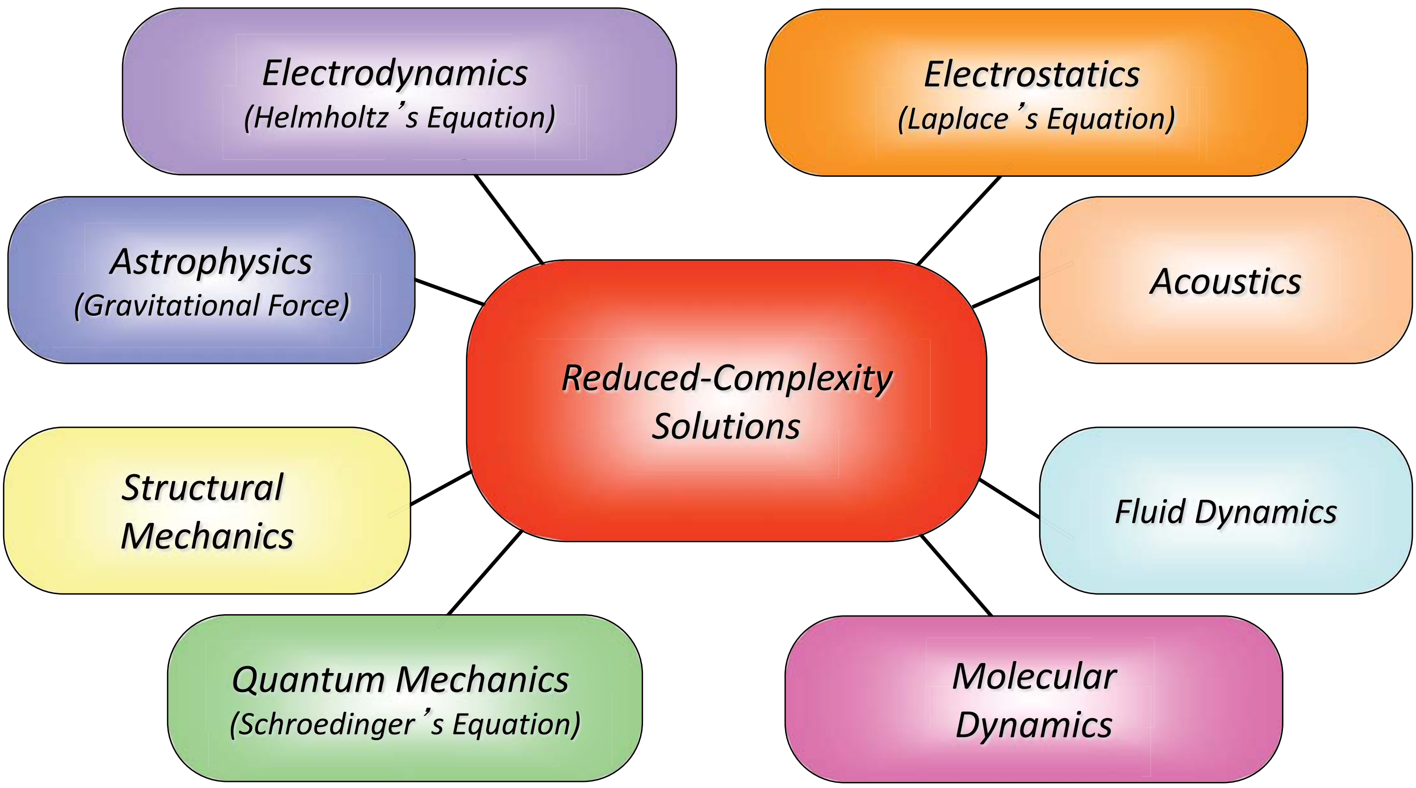
Major Parts of MLFMA and Their Computational Requirements

	Memory	
Part	Proportional to	Complexity
MVM	$\sum_{l=1}^{L} N_l[\tau(l)+1]^2$	$\mathcal{O}(N \log N)$
Radiation and Receiving Patterns	$N[\tau(1)+1]^2$	$\mathcal{O}(N)$
Translation Operators	$\sum_{l=1}^{L} d_l[\tau(l)+1]^2$	$\mathcal{O}(N)$
Near-Field Interactions	N^2/N_1	$\mathcal{O}(N)$

	Processing Time	
Part	Proportional to	Complexity
MVM	$\sum_{l=1}^{L} c_l N_l[\tau(l)+1]^2$	$\mathcal{O}(N \log N)$
Radiation and Receiving Patterns	$N[\tau(1)+1]^2$	$\mathcal{O}(N)$
Translation Operators	$\sum_{l=1}^{L} d_l[\tau(l)+1]^2$	$\mathcal{O}(N)$
Near-Field Interactions	N^2/N_1	$\mathcal{O}(N)$

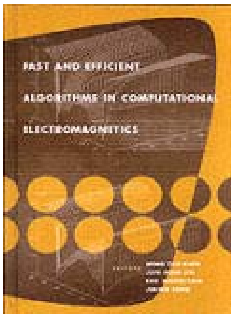
Note: c_l and d_l represent relative weights for levels $l = 1, 2, \ldots, L$.

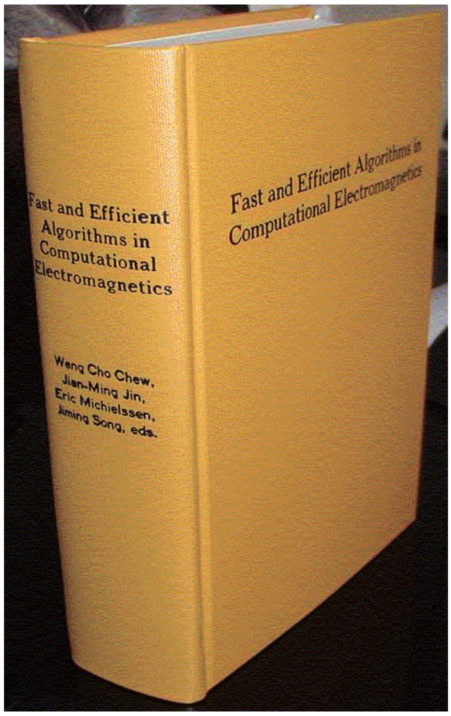
Fast Multipole Methods



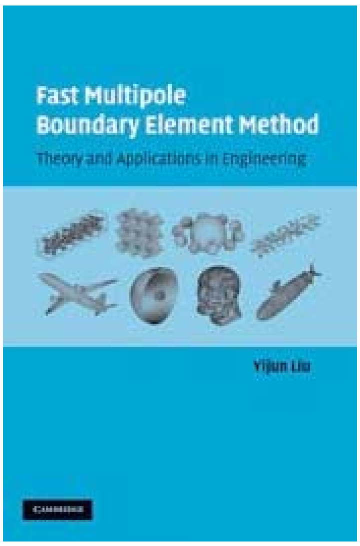
Multilevel Fast Multipole Algorithm

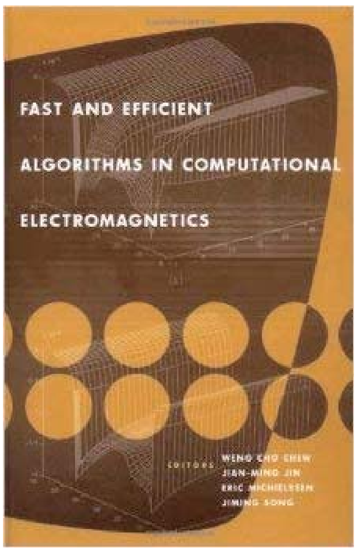
Fast and Efficient Algorithms in Computational Electromagnetics
by
W.C. Chew, J.M. Jin, E. Michielssen, J.M. Song, Eds.

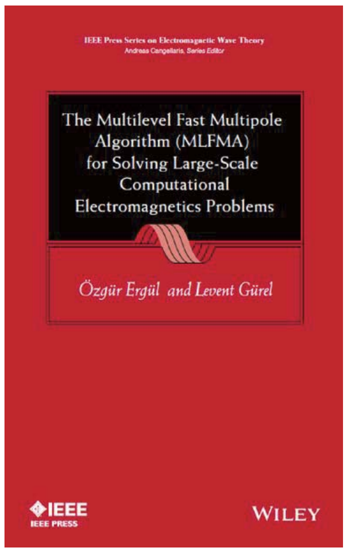




Books







Integral Equations, Fast Algorithms, and Parallelization Strategies

for the Solution of Extremely Large Problems

in Computational Electromagnetics

Prof. Levent Gürel
CEO, ABAKUS Computing Technologies
Adjunct Professor, ECE, Univ. of Illinois at Urbana-Champaign

May 2015

Parallel MLFMA

(Multilevel Fast Multipole Algorithm)

Prof. Levent Gürel
CEO, ABAKUS Computing Technologies
Adjunct Professor, ECE, Univ. of Illinois at Urbana-Champaign

May 2015

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)

Parallelization of MLFMA

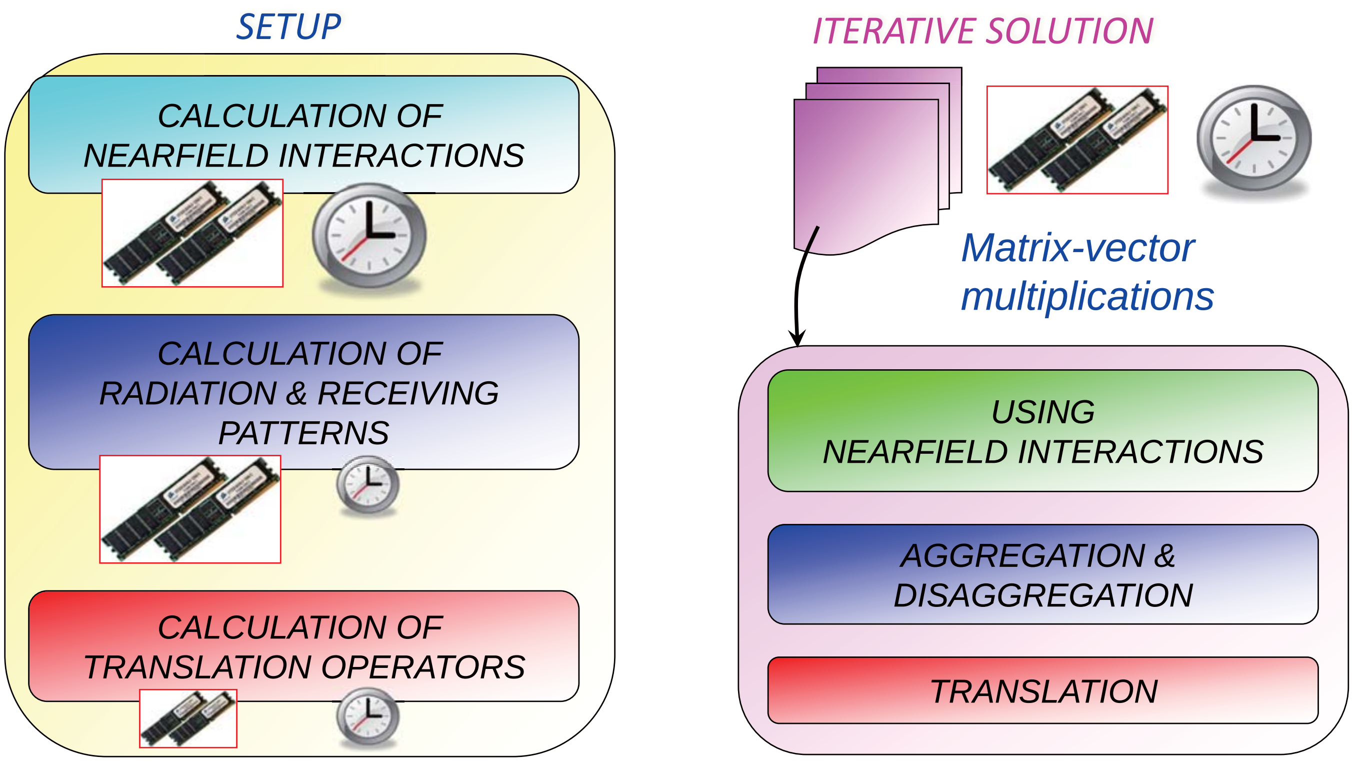
Parallelization is required

- *For the solution of realistic problems discretized with tens of millions of unknowns*
- *On relatively inexpensive computing platforms*
  - *64-128 cores*
  - *Distributed memory*
  - *Fast networks such as Infiniband*

Unfortunately, parallelization of MLFMA is not trivial!

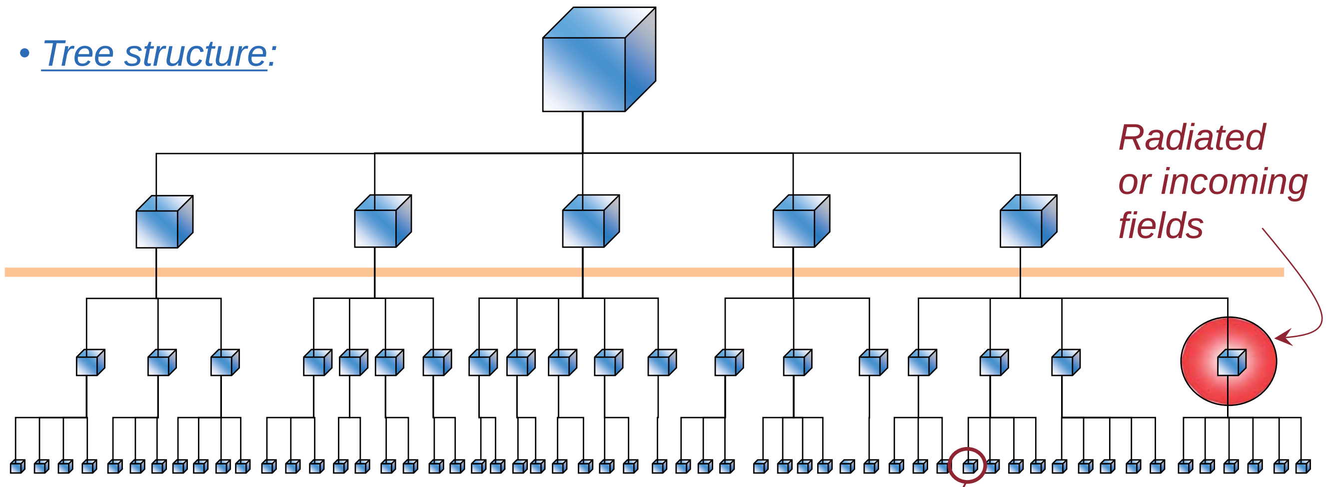
Parallel Computers

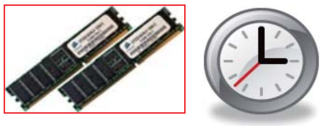
Multilevel Fast Multipole Algorithm

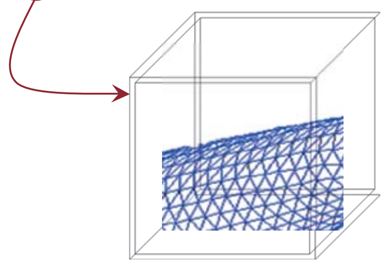


Multilevel Fast Multipole Algorithm

- *Tree structure:*

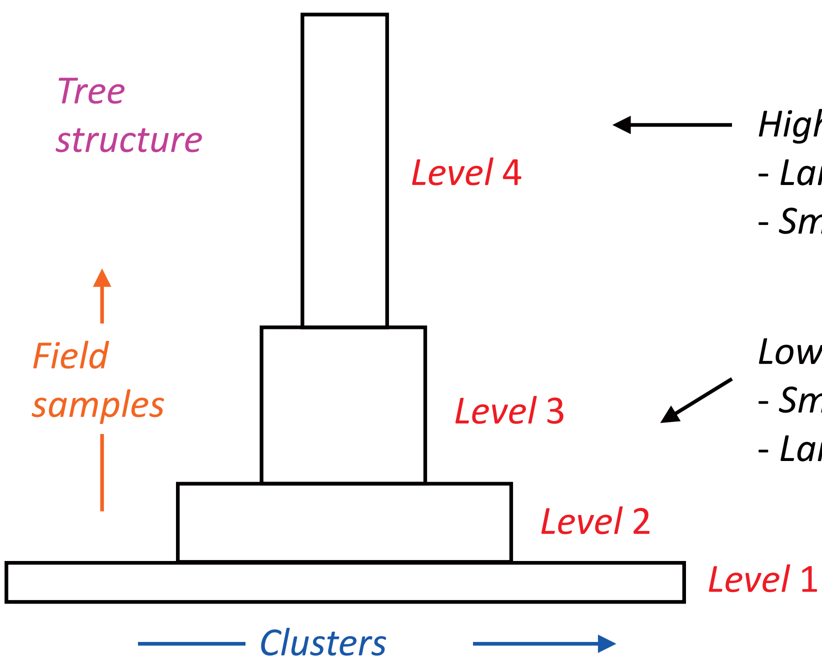






- *Complexity:* $O(N \log N)$

Multilevel Tree Structure

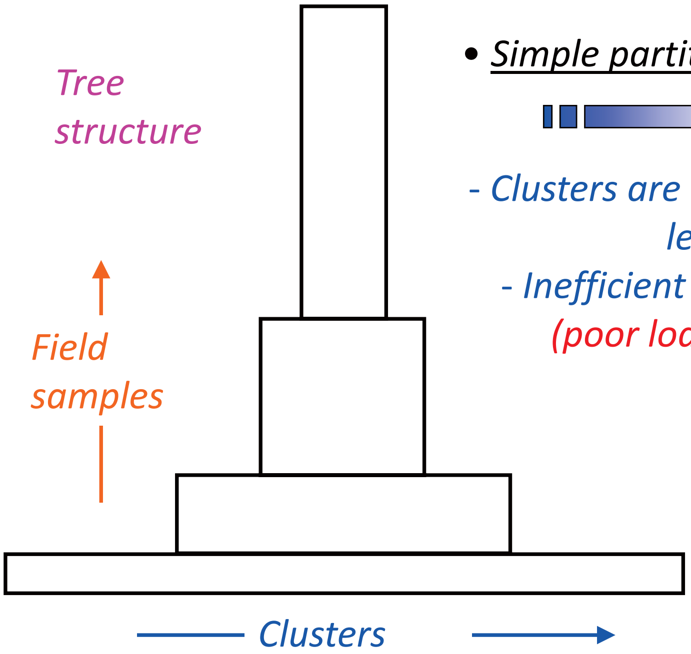


Higher levels:
- Large numbers of samples
- Small numbers of clusters

Lower levels:
- Small numbers of samples
- Large numbers of clusters

(Simple) Partitioning of Multilevel Tree

Main work: Partitioning the tree structure

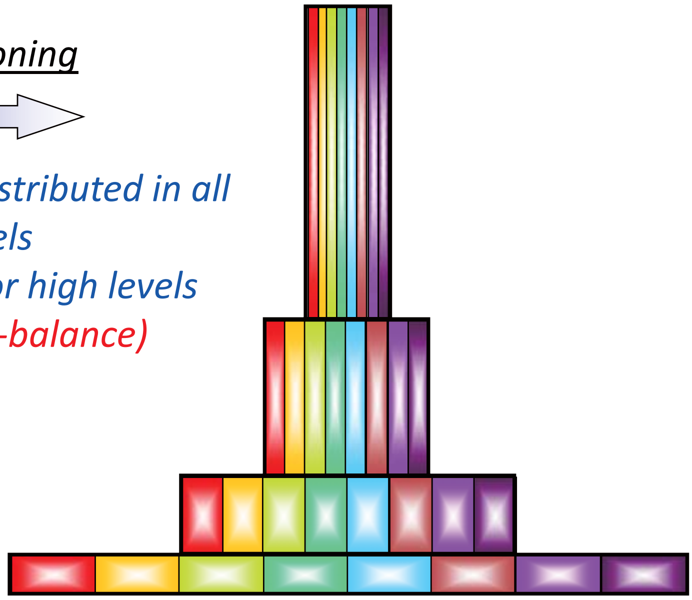


- ***Simple partitioning***

- Clusters are distributed in all levels

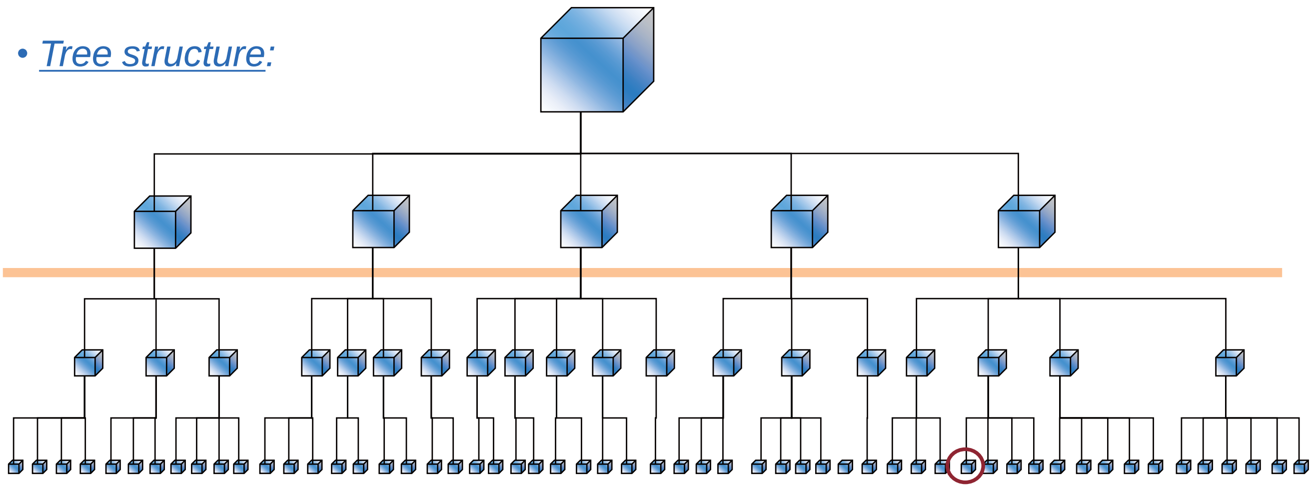
- Inefficient for high levels

(poor load-balance)



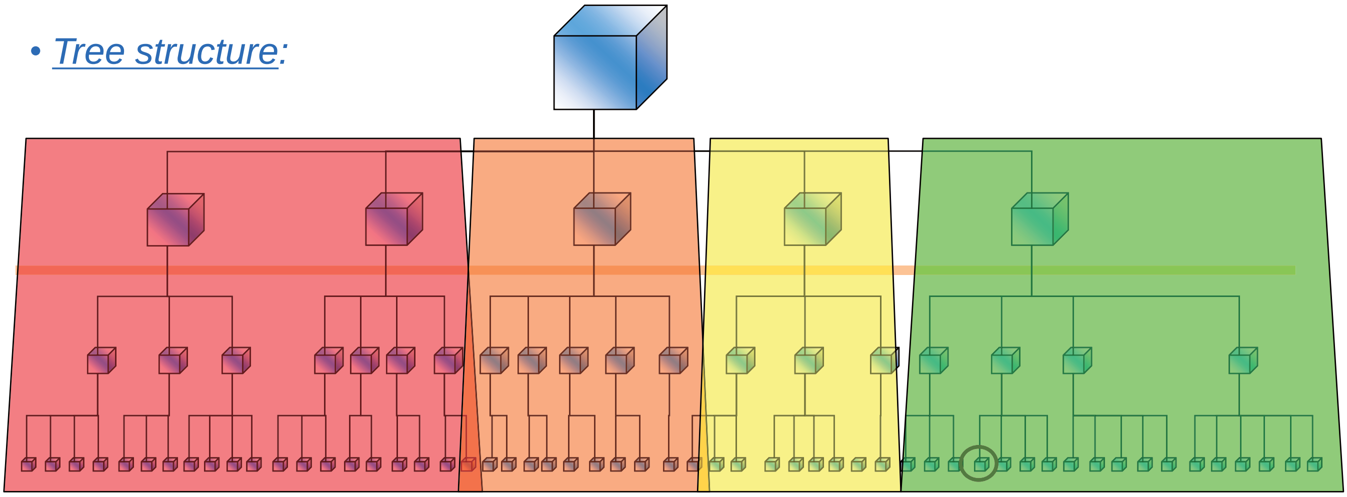
Multilevel Fast Multipole Algorithm

- *Tree structure:*



Multilevel Fast Multipole Algorithm

- *Tree structure:*



Poor load balancing!

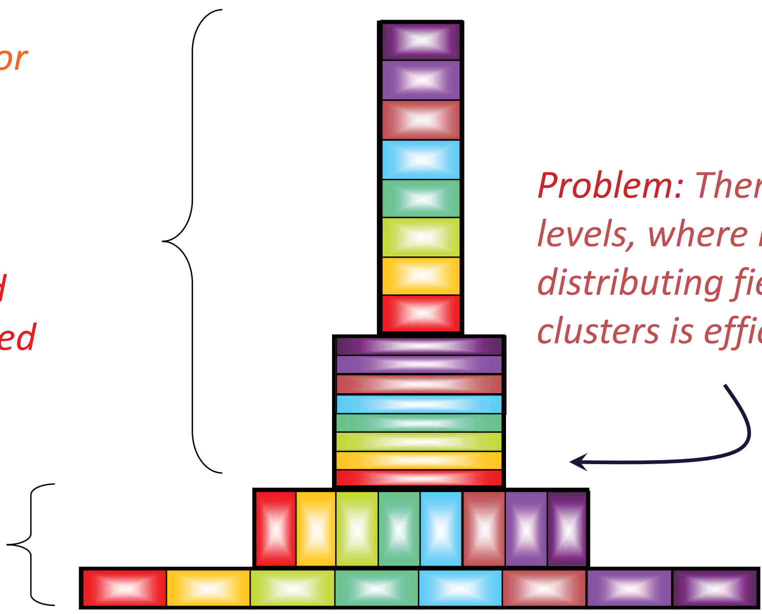
Hybrid Partitioning of Multilevel Tree
(Chew et al.)

- **Hybrid partitioning**

(improves load-balance for higher levels)

Shared levels:
- Clusters are shared
- Fields are distributed

Distributed levels:
- Clusters are distributed

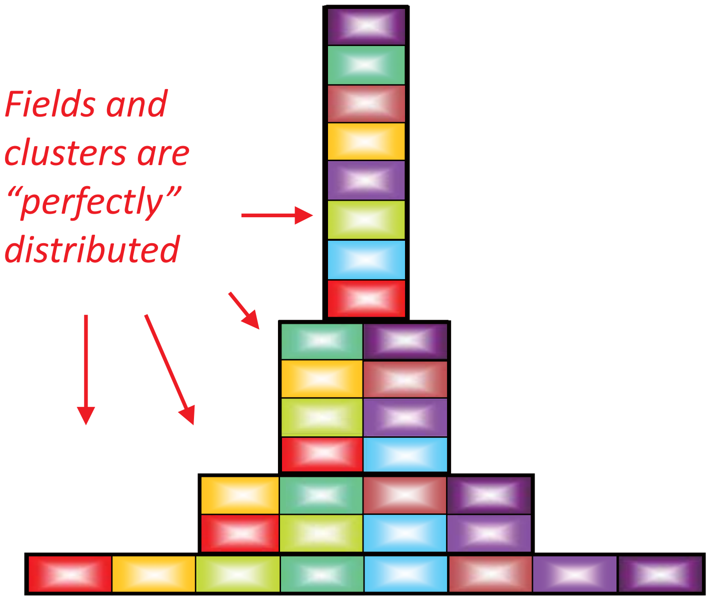


Problem: There are some levels, where neither distributing fields nor clusters is efficient

URSI AT-RASC

(Hierarchical) Partitioning of Multilevel Tree

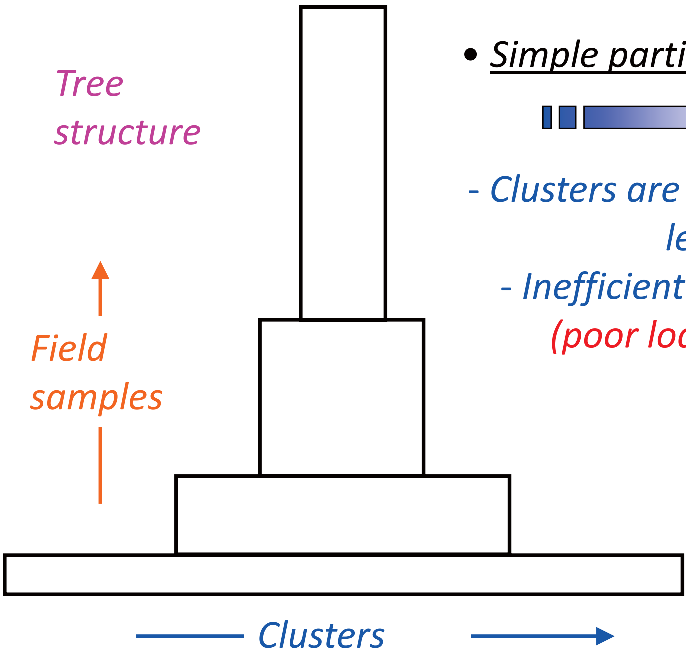
- ***Hierarchical partitioning***



URSI AT-RASC

(Simple) Partitioning of Multilevel Tree

Main work: Partitioning the tree structure

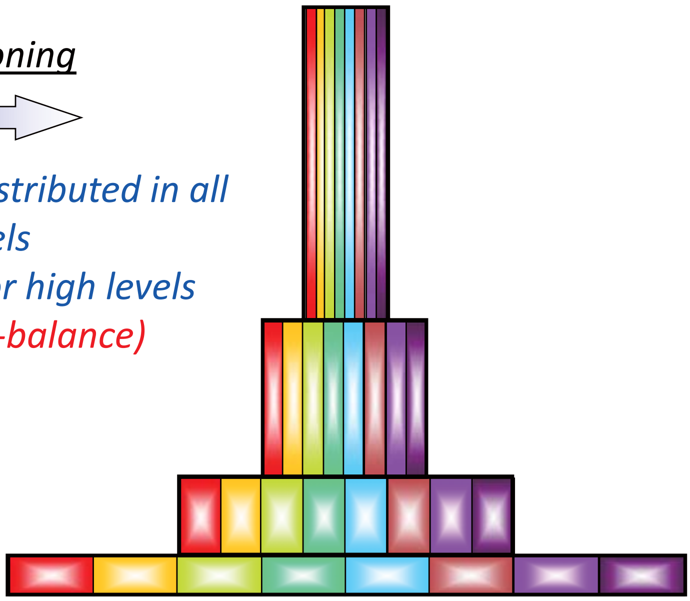


- ***Simple partitioning***

- Clusters are distributed in all levels

- Inefficient for high levels

(poor load-balance)

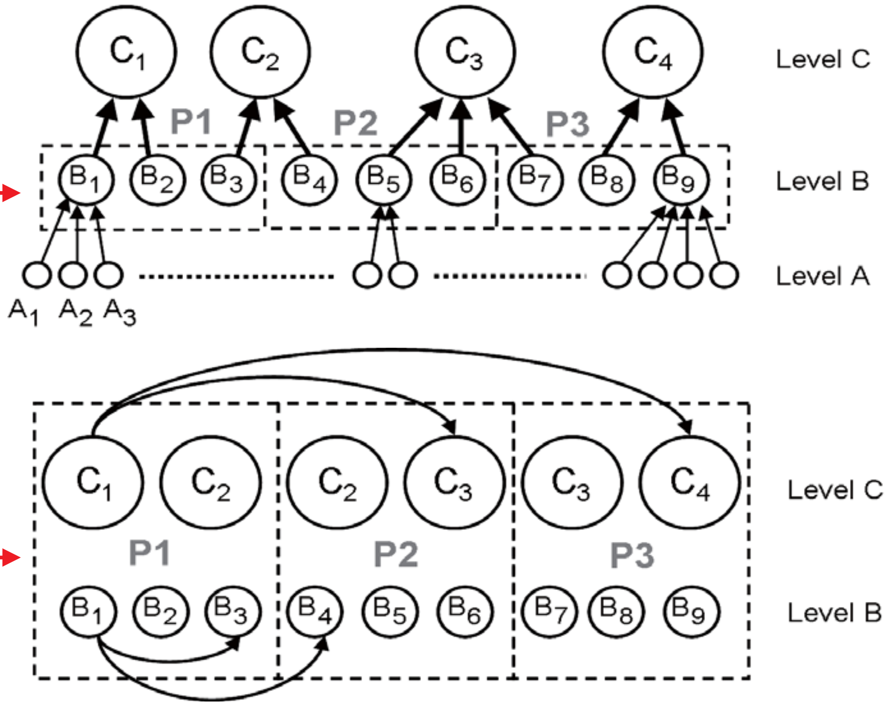


Simple Parallelization

Distributing Clusters Among Processors

Aggregations

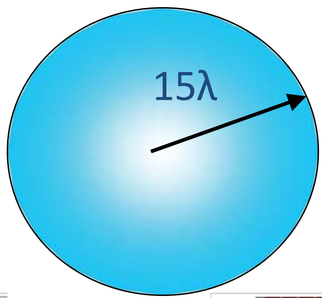
Translations

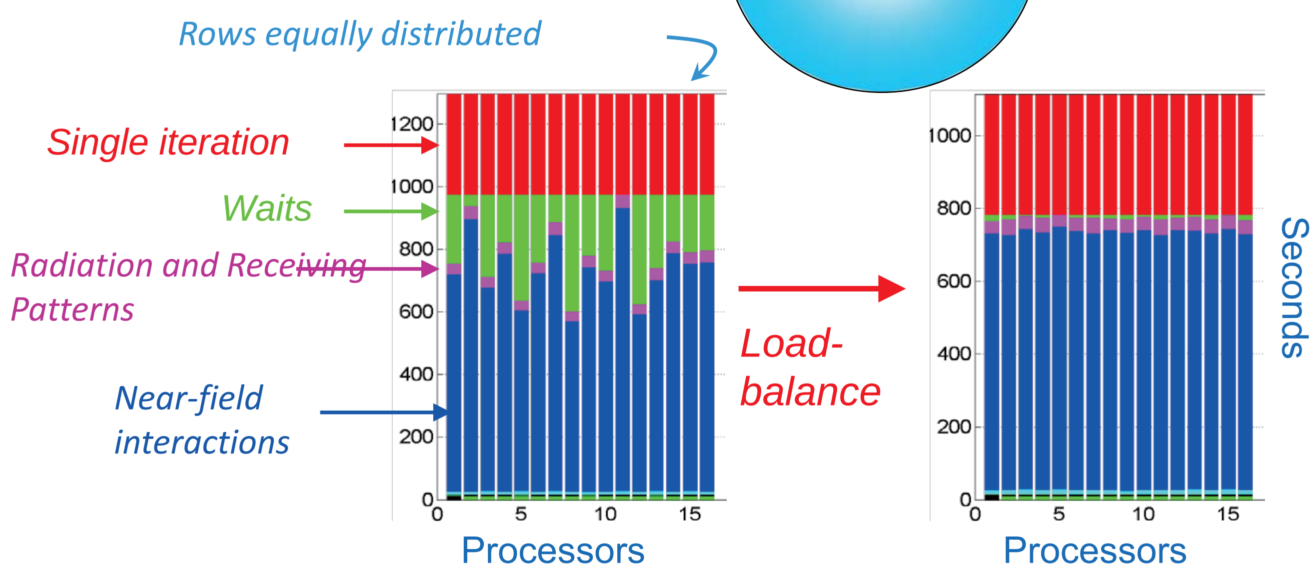


Near-Field Interactions

- Near-field partitioning

Sphere problem
(829,881 unknowns)

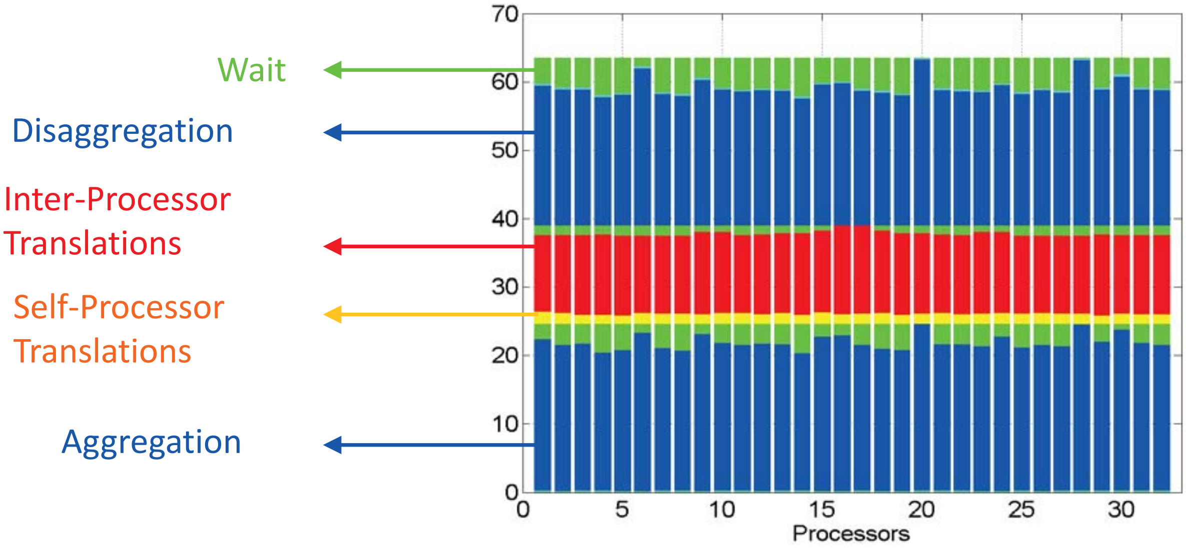




Simple Parallelization

Processing Time (Seconds) for Sphere Problem (829,881 unknowns)

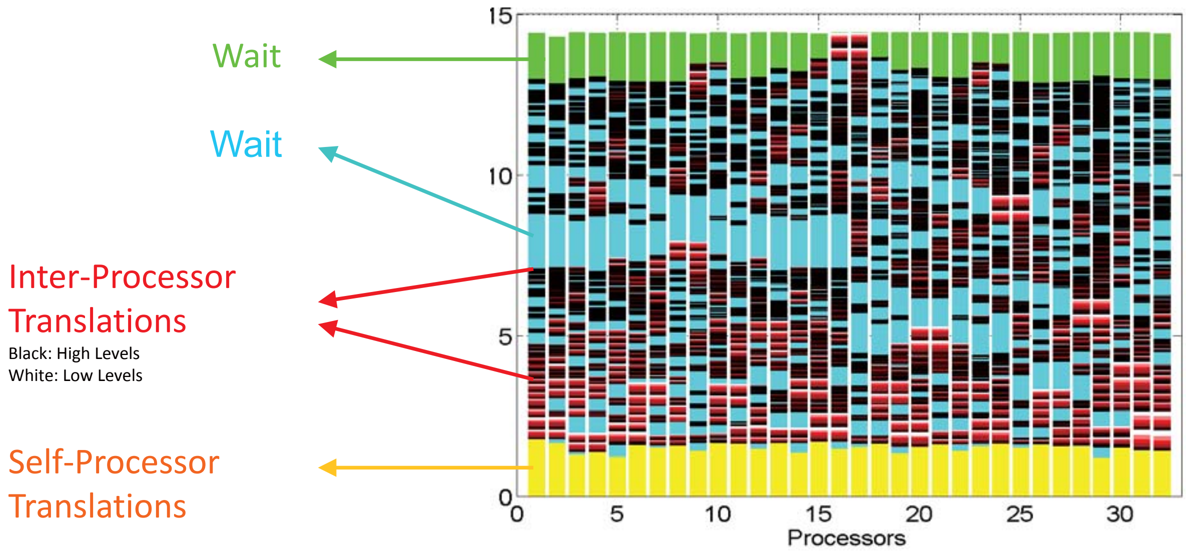
Matrix-Vector Multiplications



Simple Parallelization

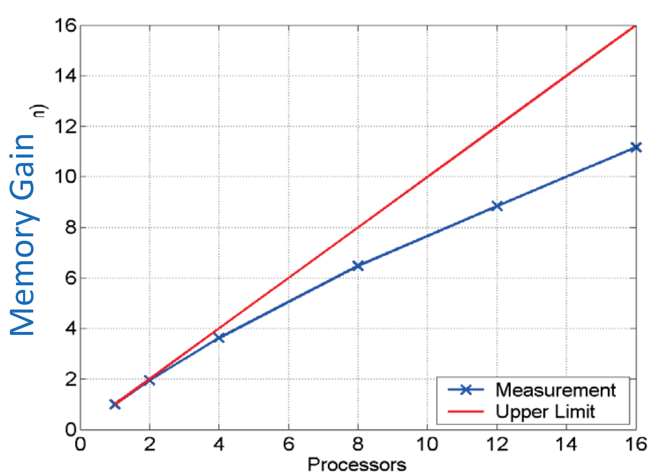
Processing Time (Seconds) for Sphere Problem (829,881 unknowns)

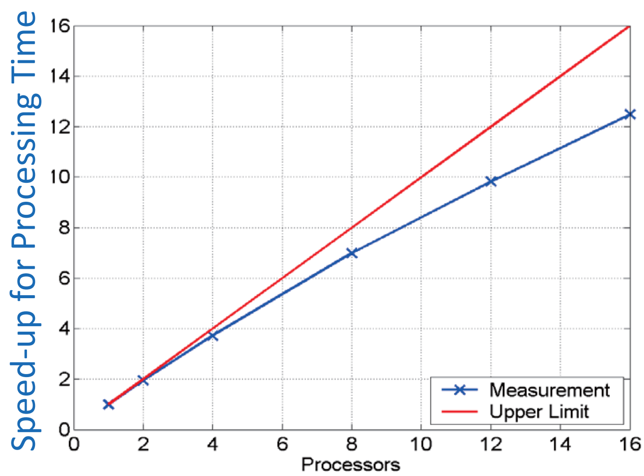
Translations



Speed-up and Gain

Sphere Problem (132,003 unknowns)

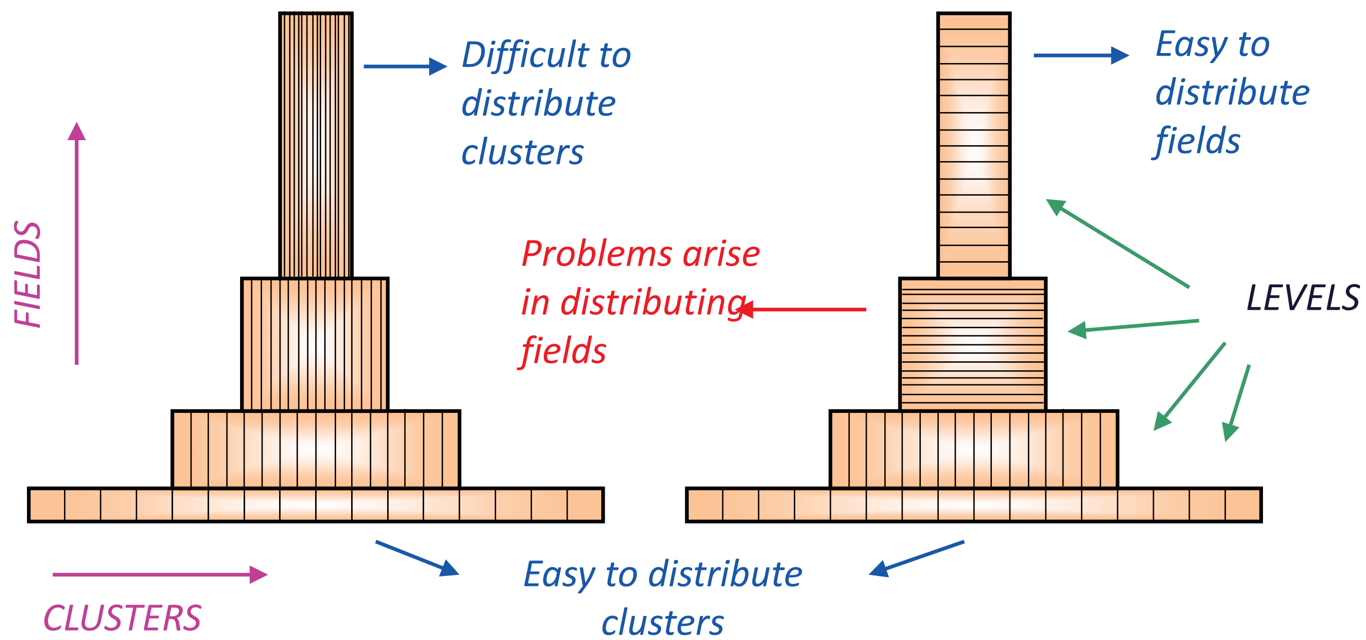




Partitioning

Simple parallellization
(All levels are distributed)

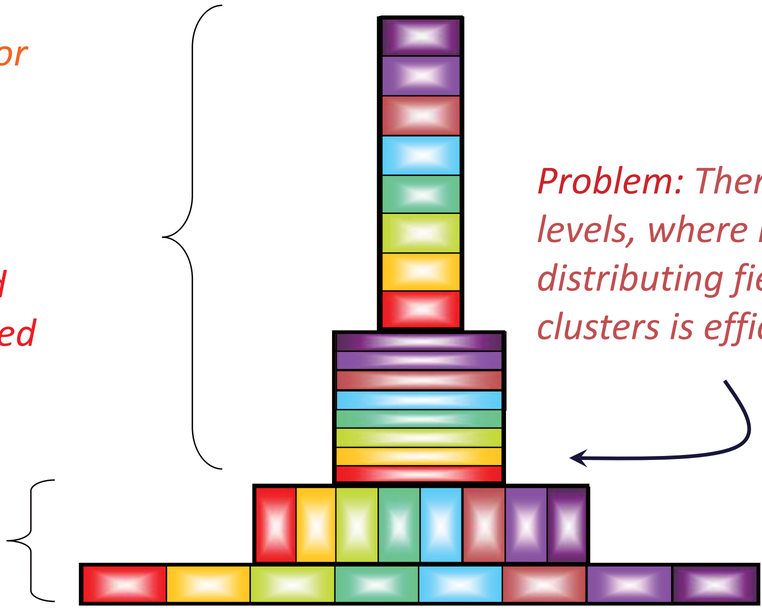
Hybrid parallellization
(Shared & distributed levels)



Hybrid Partitioning of Multilevel Tree

• *Hybrid partitioning*
(improves load-balance for higher levels)

Shared levels:
- Clusters are shared
- Fields are distributed



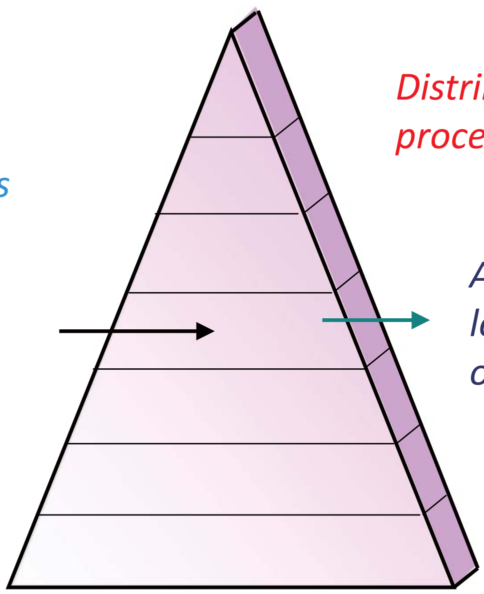
Problem: There are some levels, where neither distributing fields nor clusters is efficient

Distributed levels:
- Clusters are distributed

Far-Field Interactions

HIGH LEVELS
Small numbers of clusters
Large numbers of samples

Distribute fields among the processors



Level of Distribution (LoD) between shared and distributed levels

Apply load-balancing in this level by considering bunch of subclusters below

LOW LEVELS
Large numbers of clusters
Small numbers of samples

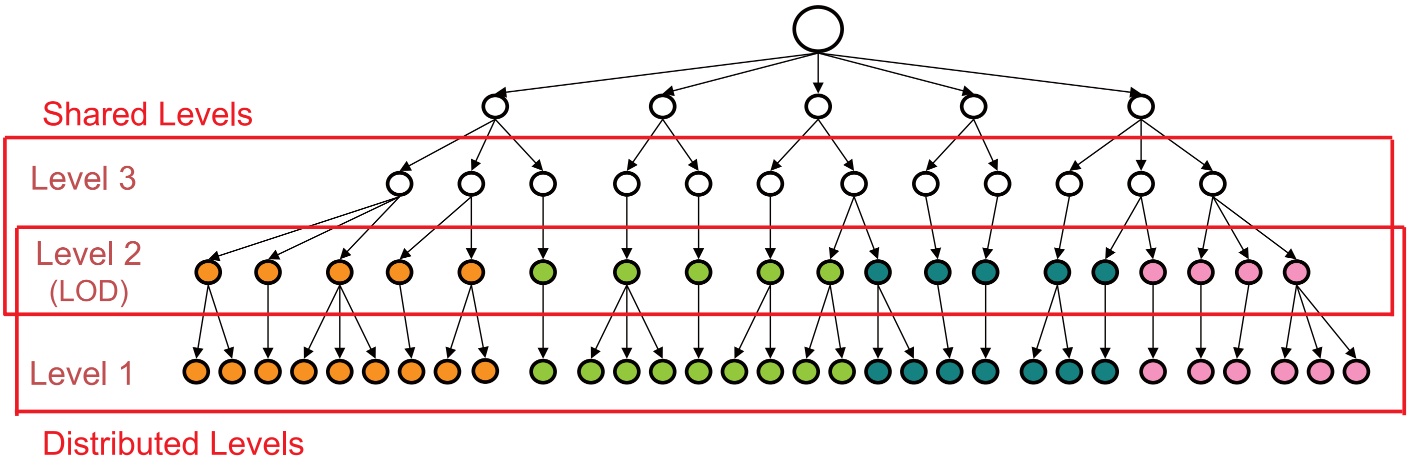
Distribute clusters among the processors

S. Velamparambil and W. C. Chew, "Analysis and performance of a distributed memory multilevel fast multipole algorithm," IEEE Trans. Antennas Propag., vol. 53, pp. 2719–2727, Aug. 2005.

Hybrid Parallelization

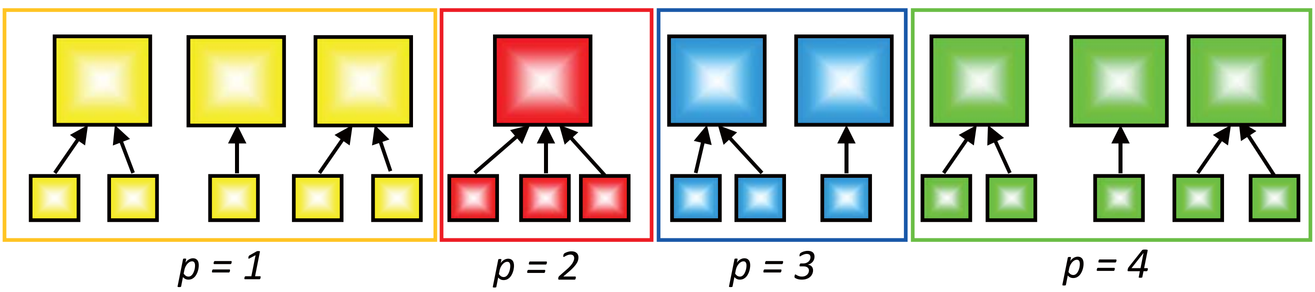
- For Low Levels of MLFMA: Distribute Clusters Among Processors (Distributed Levels)
- For High Levels of MLMFA: Distribute Fields Among the Processors (Shared Levels)

S. Velamparambil and W. C. Chew, "Analysis and performance of a distributed memory multilevel fast multipole algorithm," *IEEE Trans. Antennas Propag.*, vol. 53, pp. 2719-2727, Aug. 2005.



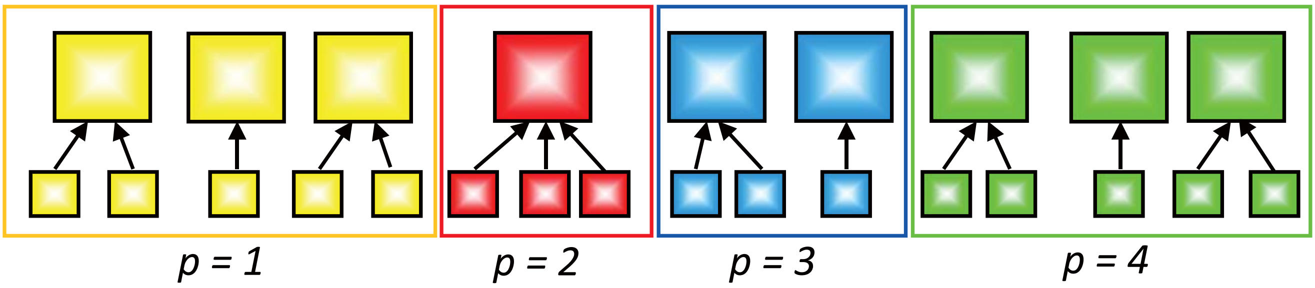
Aggregation / Disaggregation

- *Aggregation and disaggregation in distributed levels*

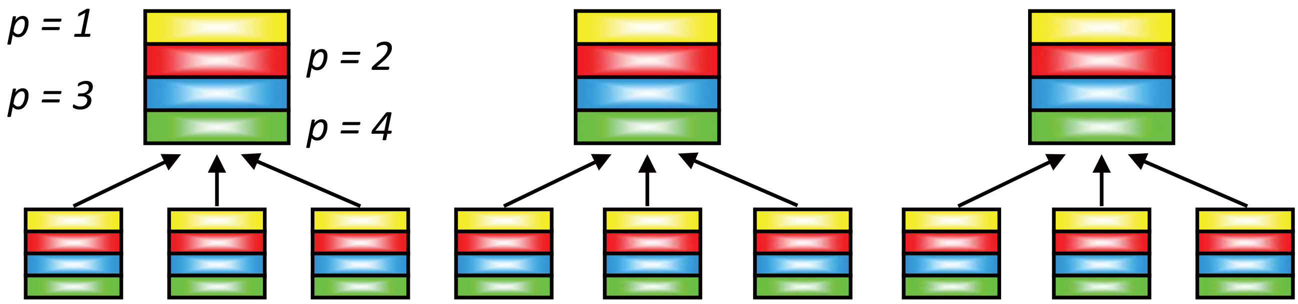


Aggregation / Disaggregation

- *Aggregation and disaggregation in distributed levels*

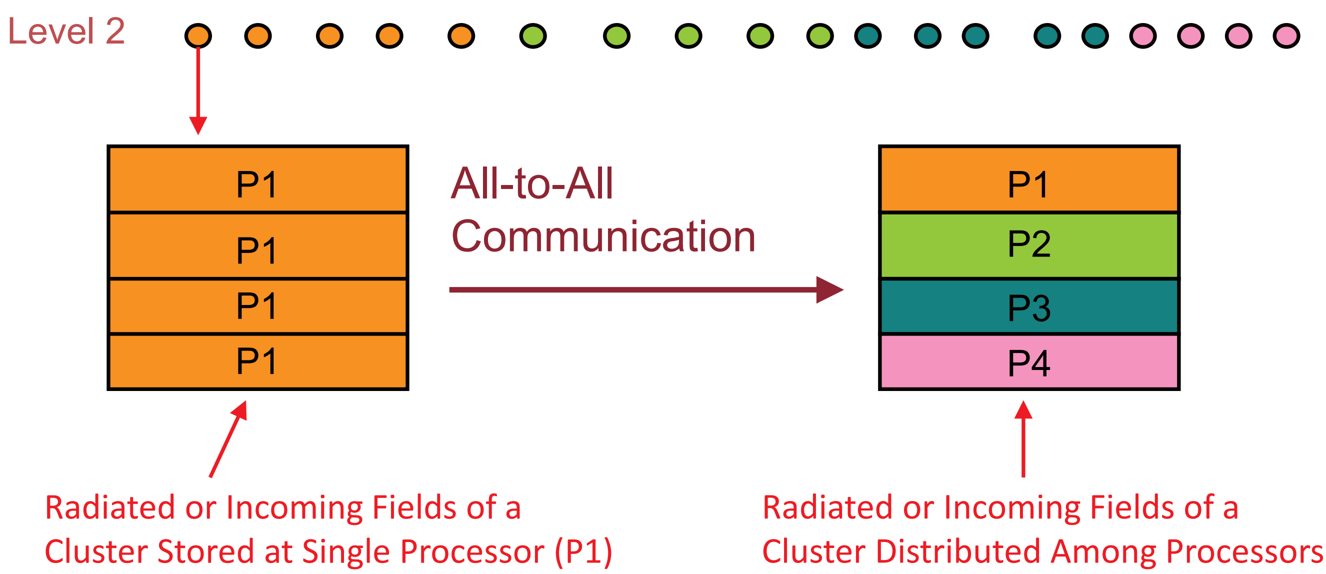


- *Aggregation and disaggregation in shared levels*

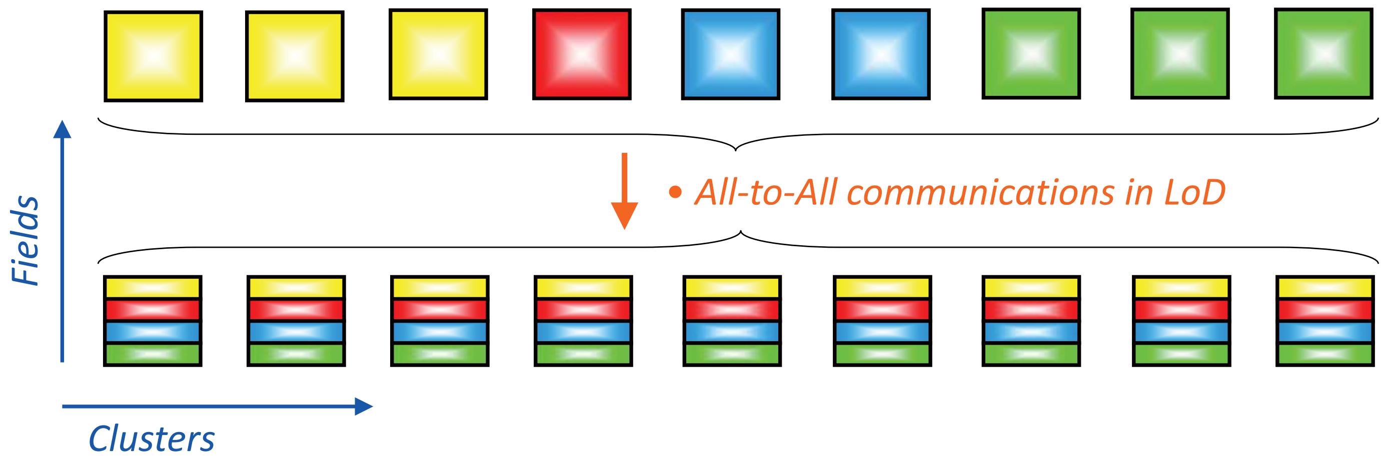


Hybrid Parallelization

Level of Distribution (LoD):
Connection Between Distributed and Shared Levels



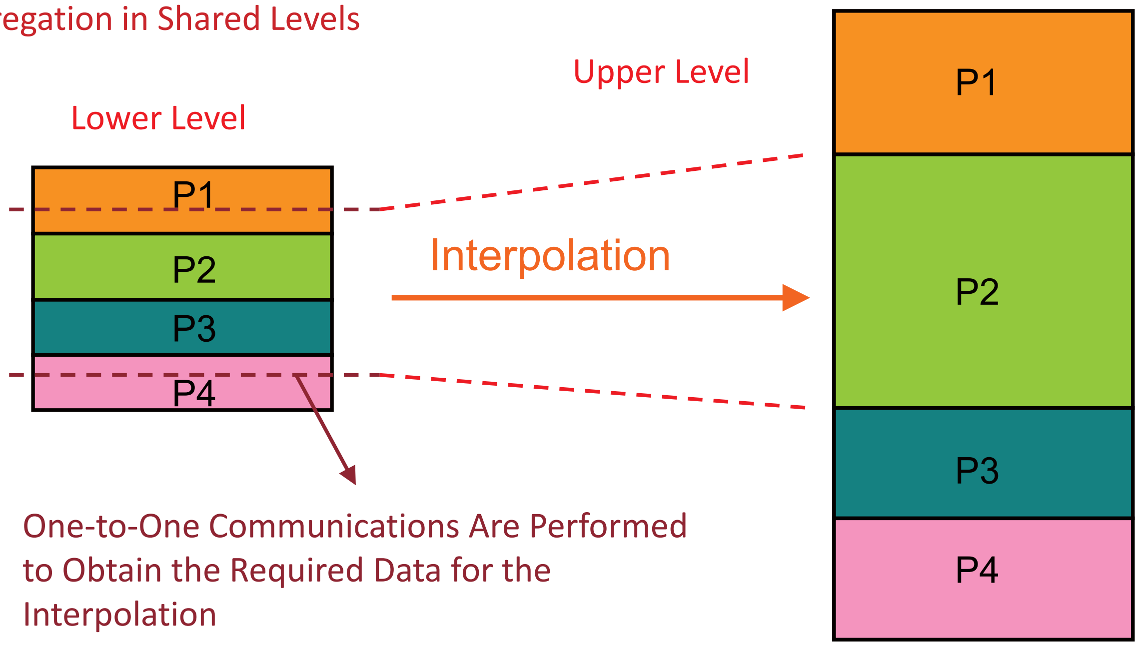
Aggregation / Disaggregation



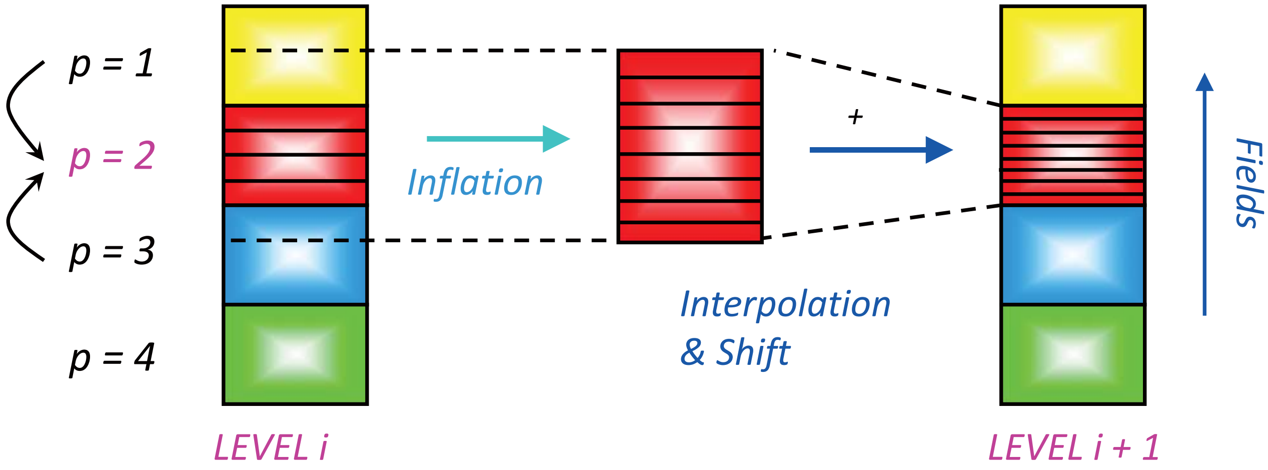
- *Aggregation and disaggregation in the distributed levels are communication-free (no communications).*
- *In the shared levels, fields are partitioned along field samples.*
- *Aggregation and disaggregation in the shared levels require one-to-one communications*

Hybrid Parallelization

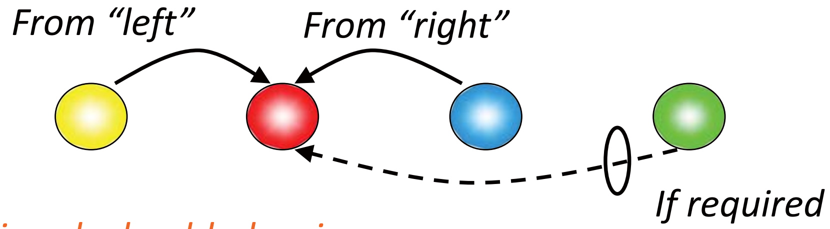
Aggregation in Shared Levels



Aggregation / Disaggregation



- *Data to p = 2*

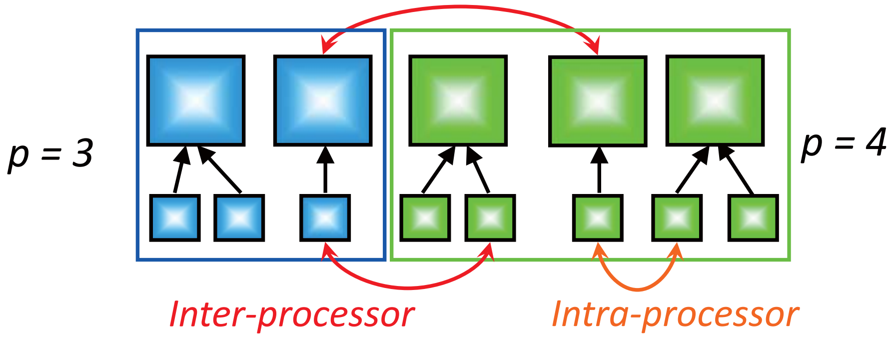


- *Reduce communications by load-balancing*

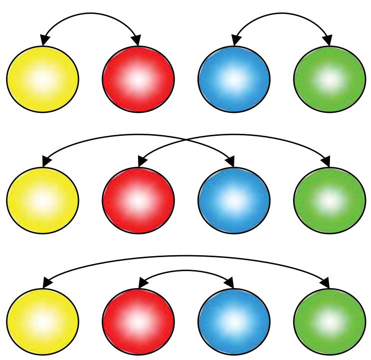
Translation

- *Distributed levels*

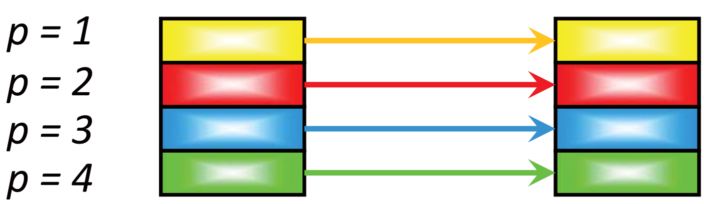
One-to-one communications are required



- *Processor pairing*



- *Shared Levels (Communication-free)*



Communications

USING NEARFIELD INTERACTIONS
- *All-to-One & One-to-All*

DISTRIBUTED AGGREGATION
- *All-to-All*

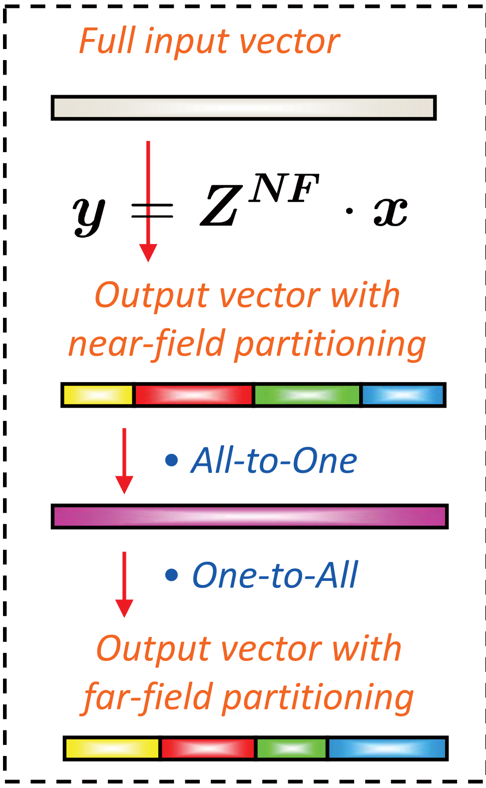
SHARED AGGREGATION
- *One-to-One*

DISTRIBUTED TRANSLATION
- *One-to-One*

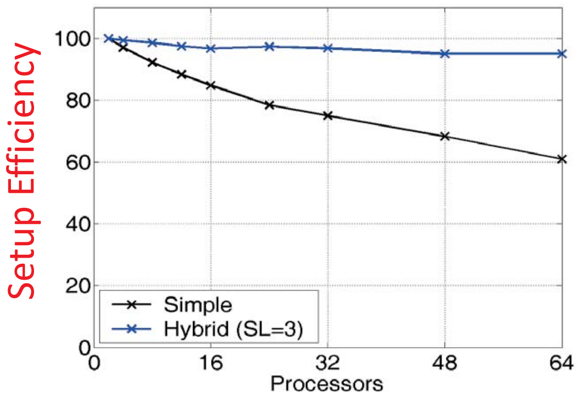
SHARED TRANSLATION

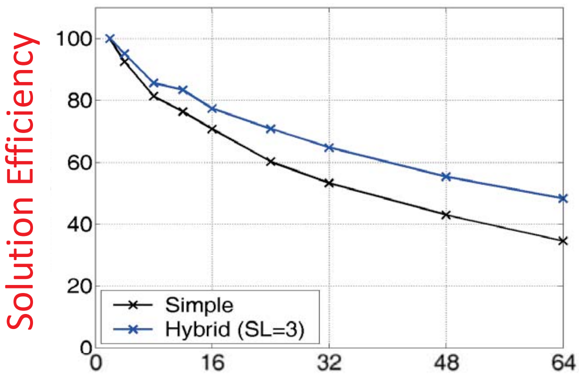
SHARED DISAGGREGATION
- *One-to-One*
- *All-to-All*

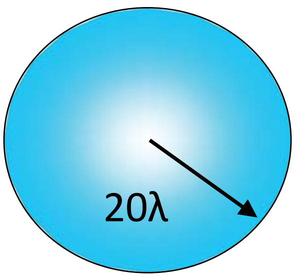
DISTRIBUTED DISAGGREGATION



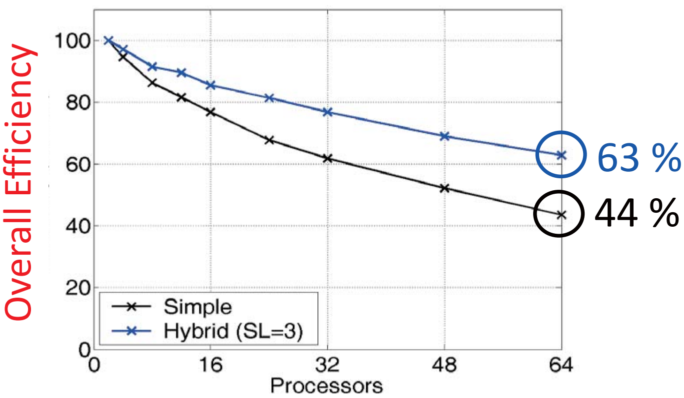
Efficiency Results





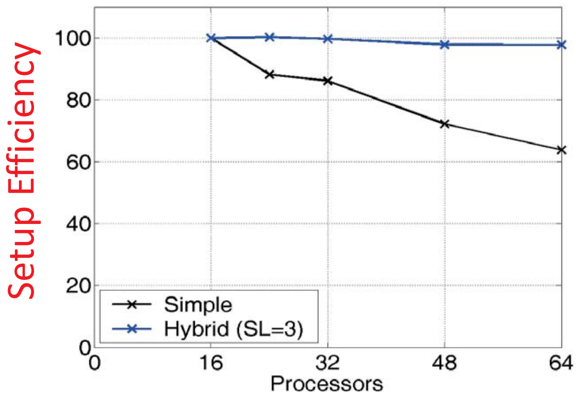


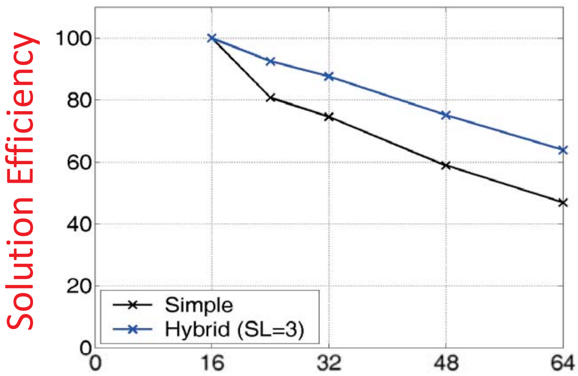
1,462,854 unknowns

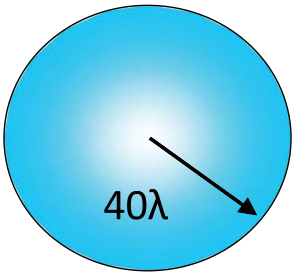


Intel Xeon 5355 processors
Infiniband network

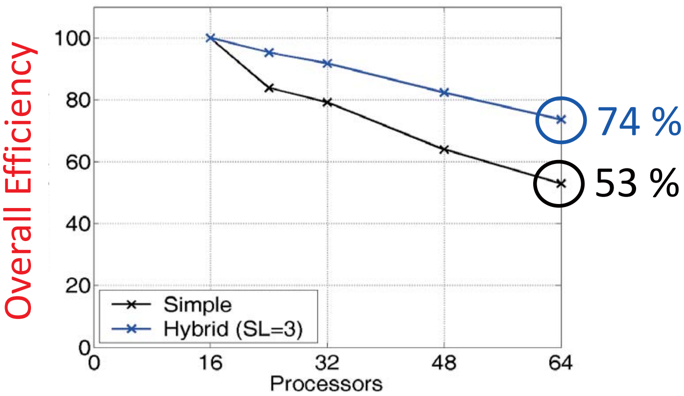
Efficiency Results





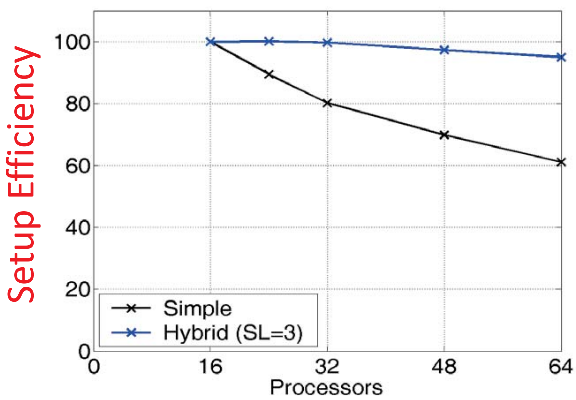


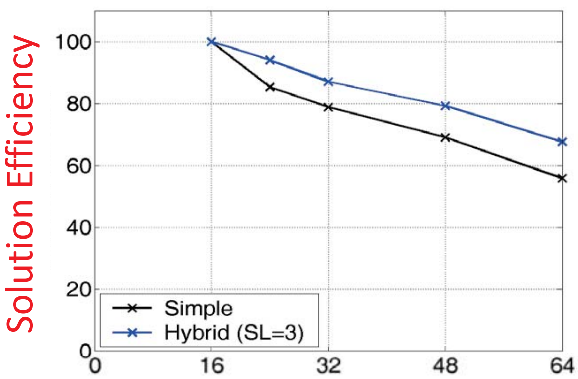
5,851,416 unknowns

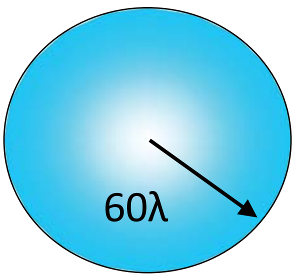


Intel Xeon 5355 processors
Infiniband network

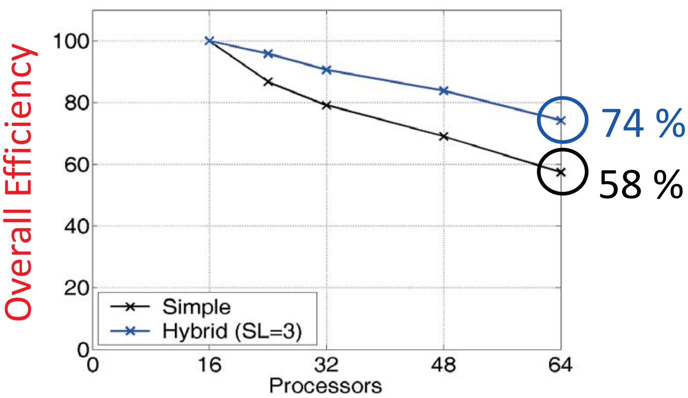
Efficiency Results







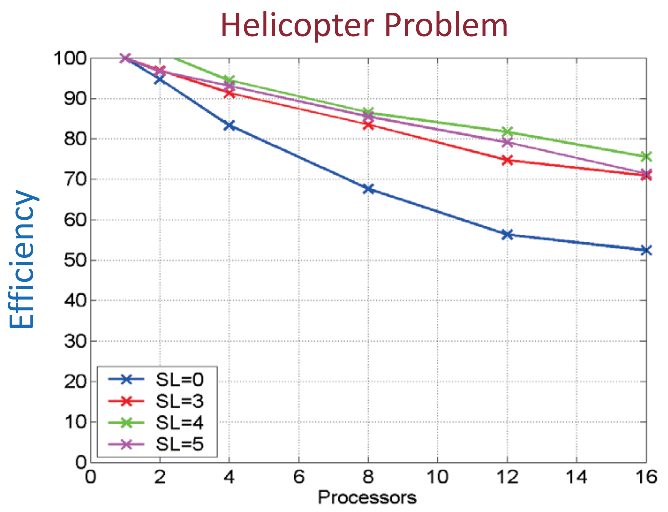
13,278,096 unknowns

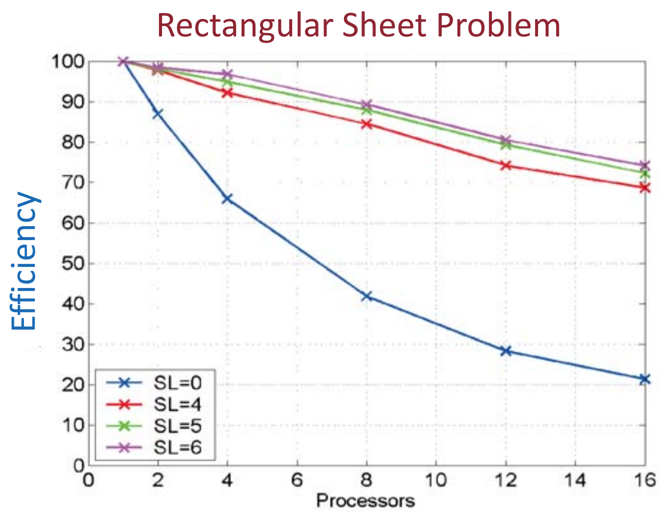


Intel Xeon 5355 processors
Infiniband network

Hybrid Parallelization

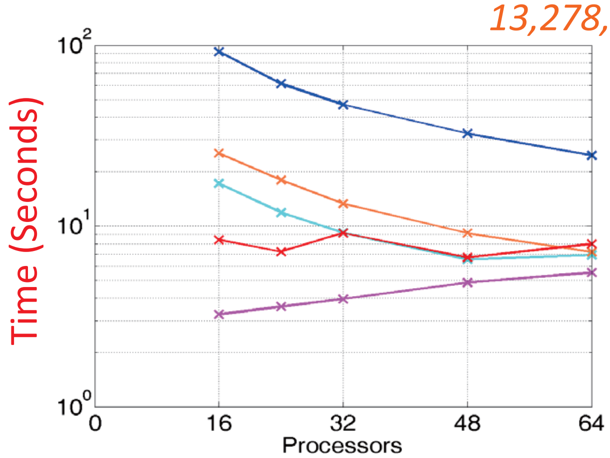
Efficiency for the Overall Processing Time

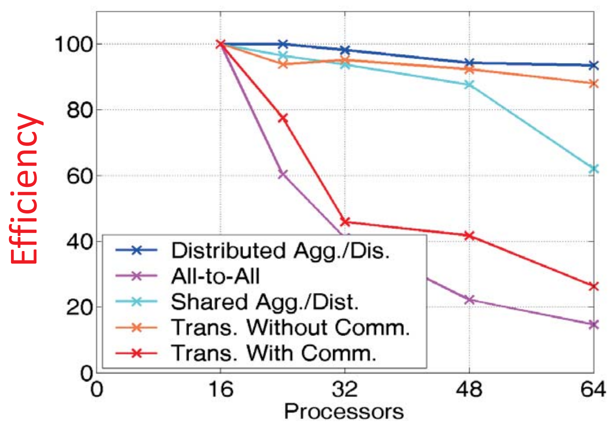




Efficiency Results

13,278,096 unknowns

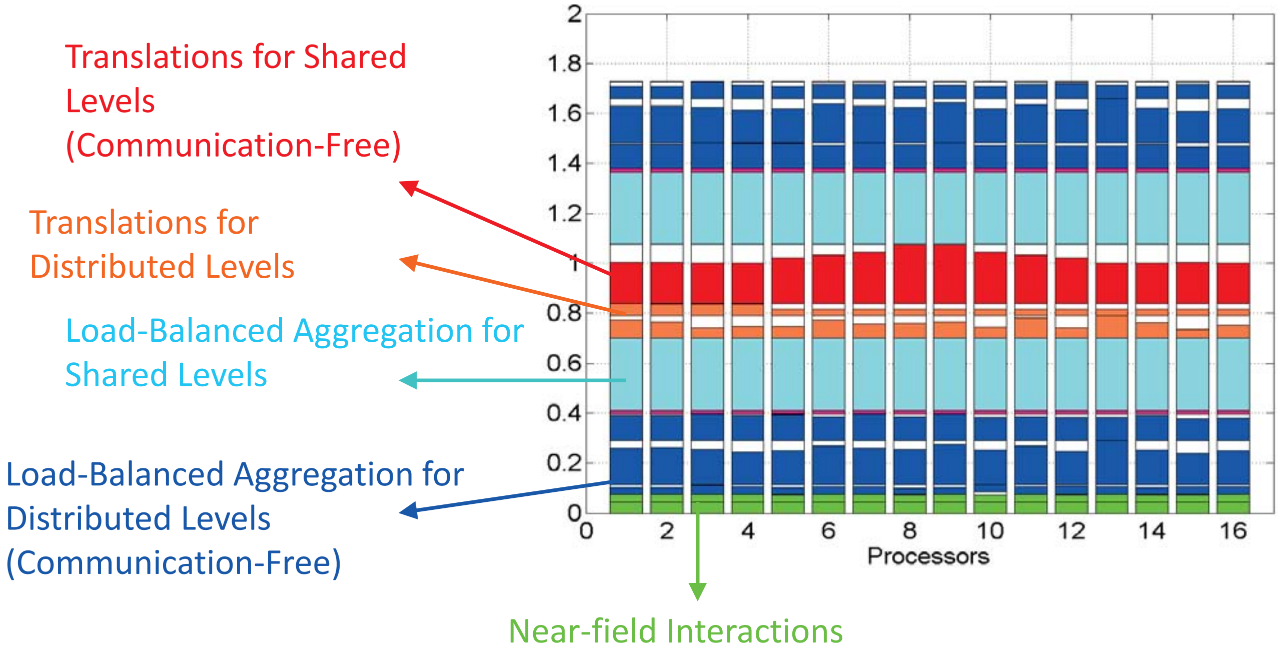




- *Translations with communications (some of those in distributed levels) are problematic.*
  Increase number of shared layers?
- *Aggregations/disaggregations in the shared levels are also problematic, when the number of processors is large and the number of samples is small.*

Hybrid Parallelization

Processing Time (Seconds) for Helicopter Problem (117,366 unknowns)
Matrix-Vector Multiplications



Hybrid Parallelization

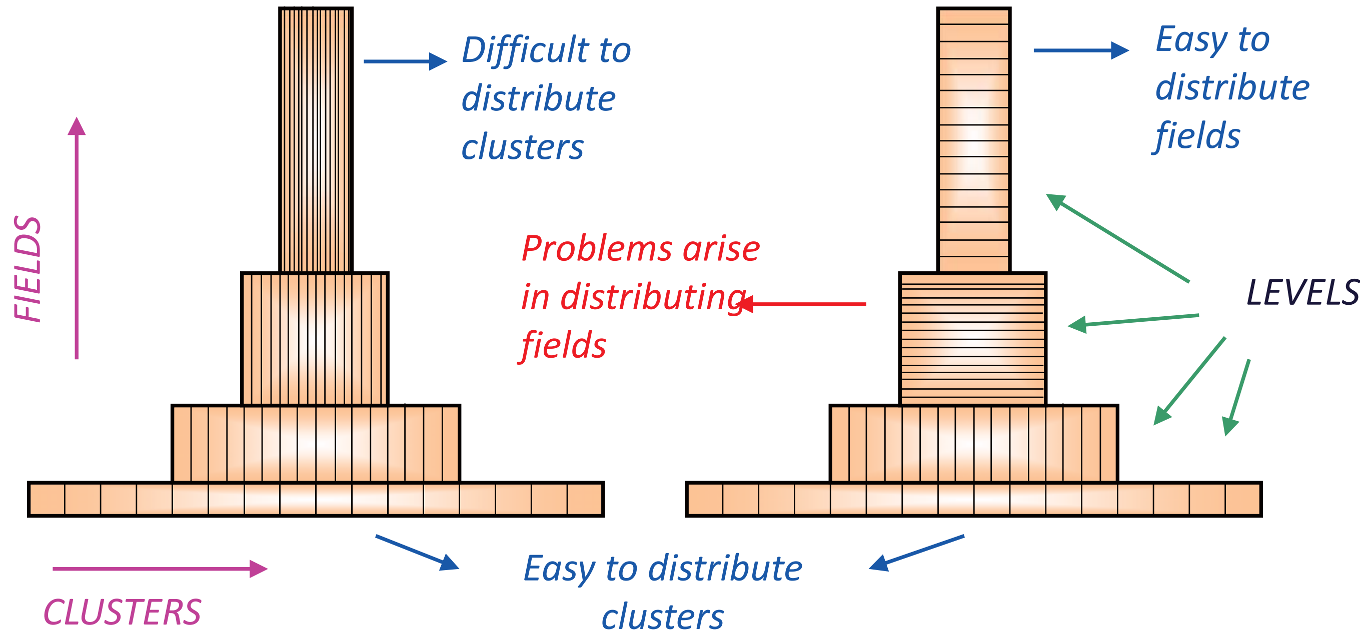
Steps of Efficient Parallelization for MLFMA

- Apply a Load-Balancing Algorithm for Near-Field Setup
- Divide the Levels into Distributed and Shared Layers
- For Distributed Levels, Apply a Load-Balancing Algorithm to Distribute Clusters Among Processors
- Perform All-to-All Communications to Pass from Distributed Levels to Shared Levels
- For Shared Levels, Apply a Load-Balancing Algorithm to Distribute Fields Among Processors
- For Translations in Distributed Levels, Apply a Communication Algorithm to Control the Data Traffic

Partitioning

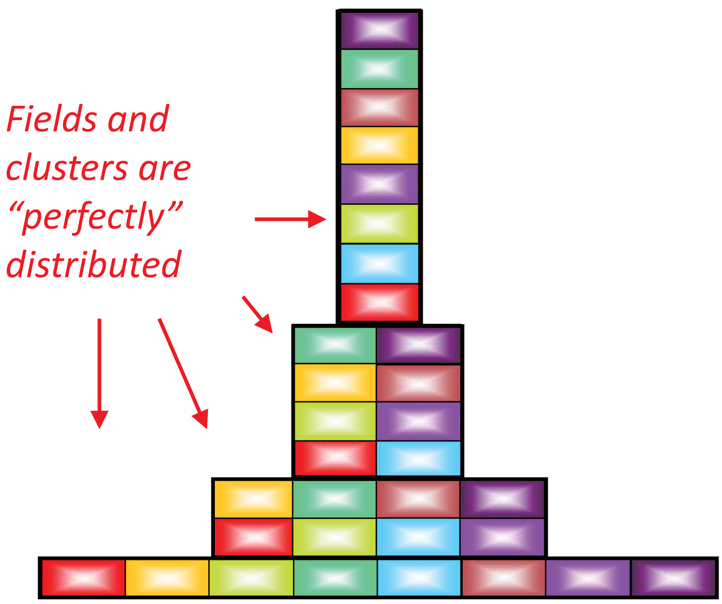
Simple parallellization
(All levels are distributed)

Hybrid parallellization
(Shared & distributed levels)



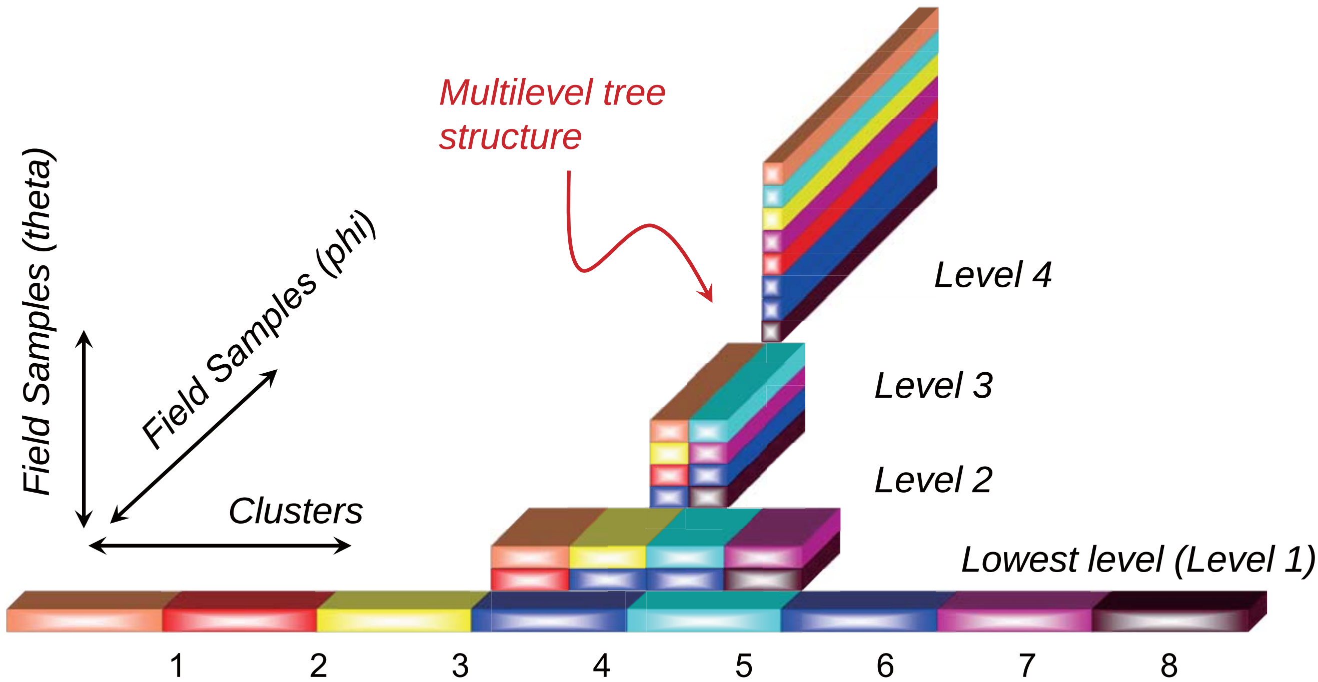
Partitioning of the Tree Structure

Hierarchical Partitioning



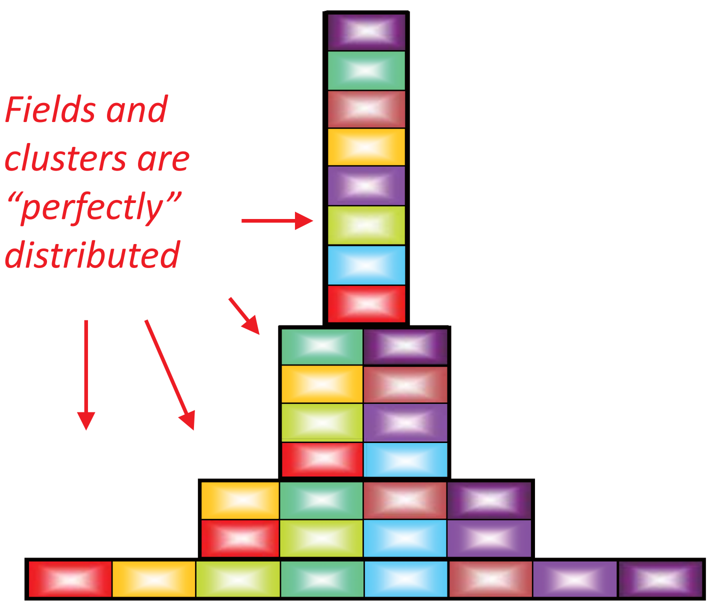
Hierarchical Parallelization

- Hierarchical Partitioning: Fields and clusters are distributed simultaneously

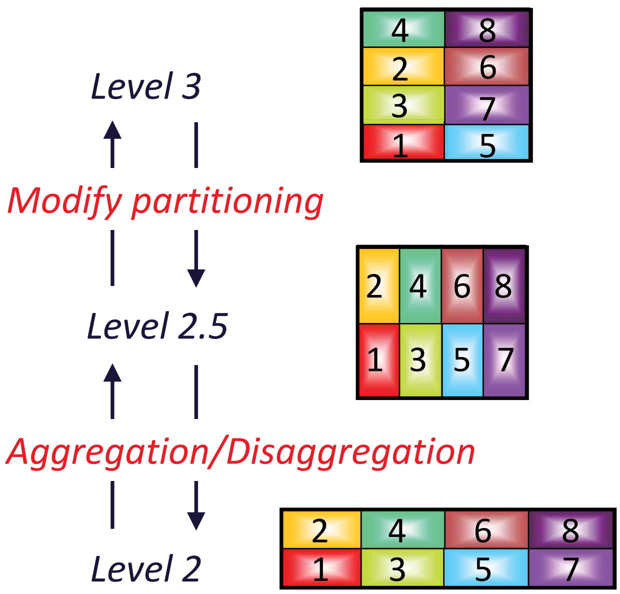


(Hierarchical) Partitioning of Multilevel Tree

- Hierarchical partitioning



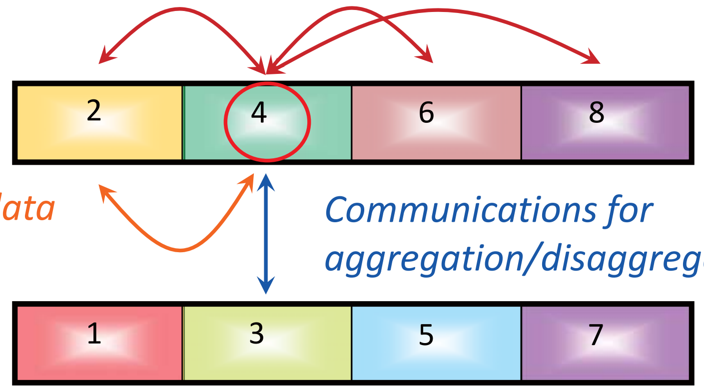
- Define intermediate levels



Communications

Consider
- *Level 2*
- *Process(or) 4*

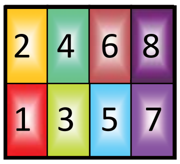
Communications for translations



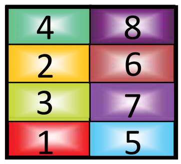
Communications for data exchange

Communications for aggregation/disaggregation

Level 2.5



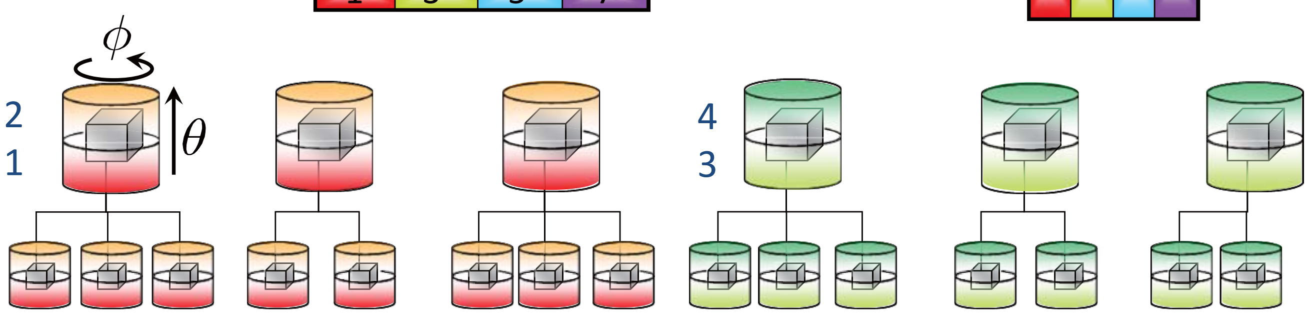
Modify partitioning



Level 3

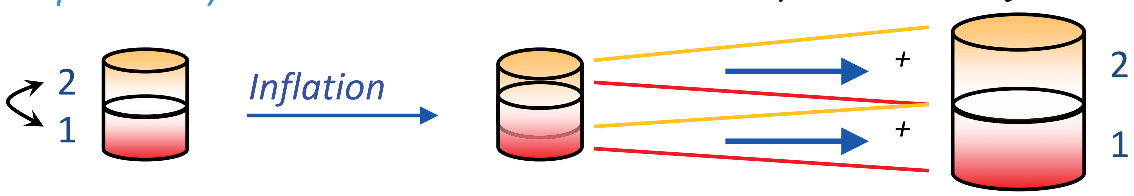
Aggregation

- *Aggregation*



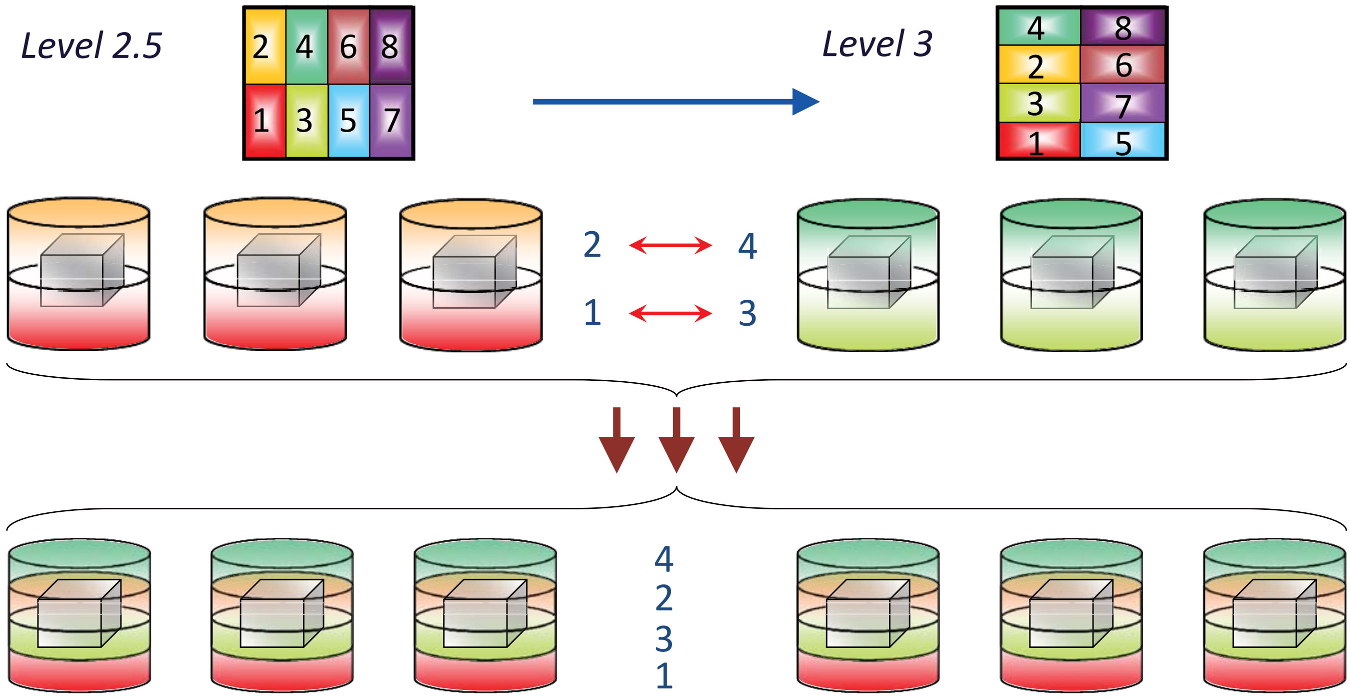
- *One-to-one communications are required (for interpolations)*

Interpolation & Shift



Data Exchange

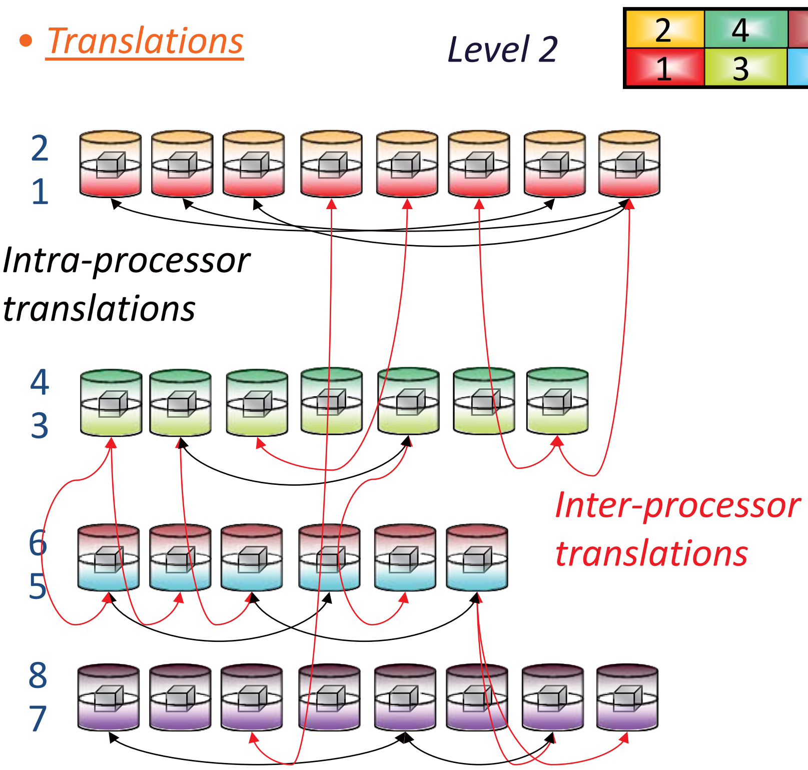
- *Data exchange to modify the partitioning*



Translation

Translation

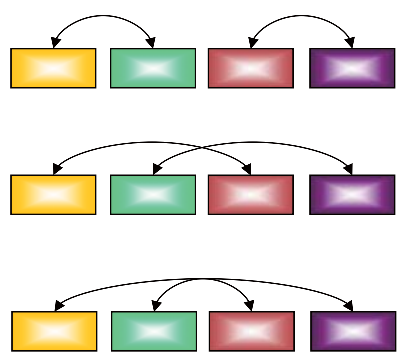
- *Translations*



- *Possible communications*

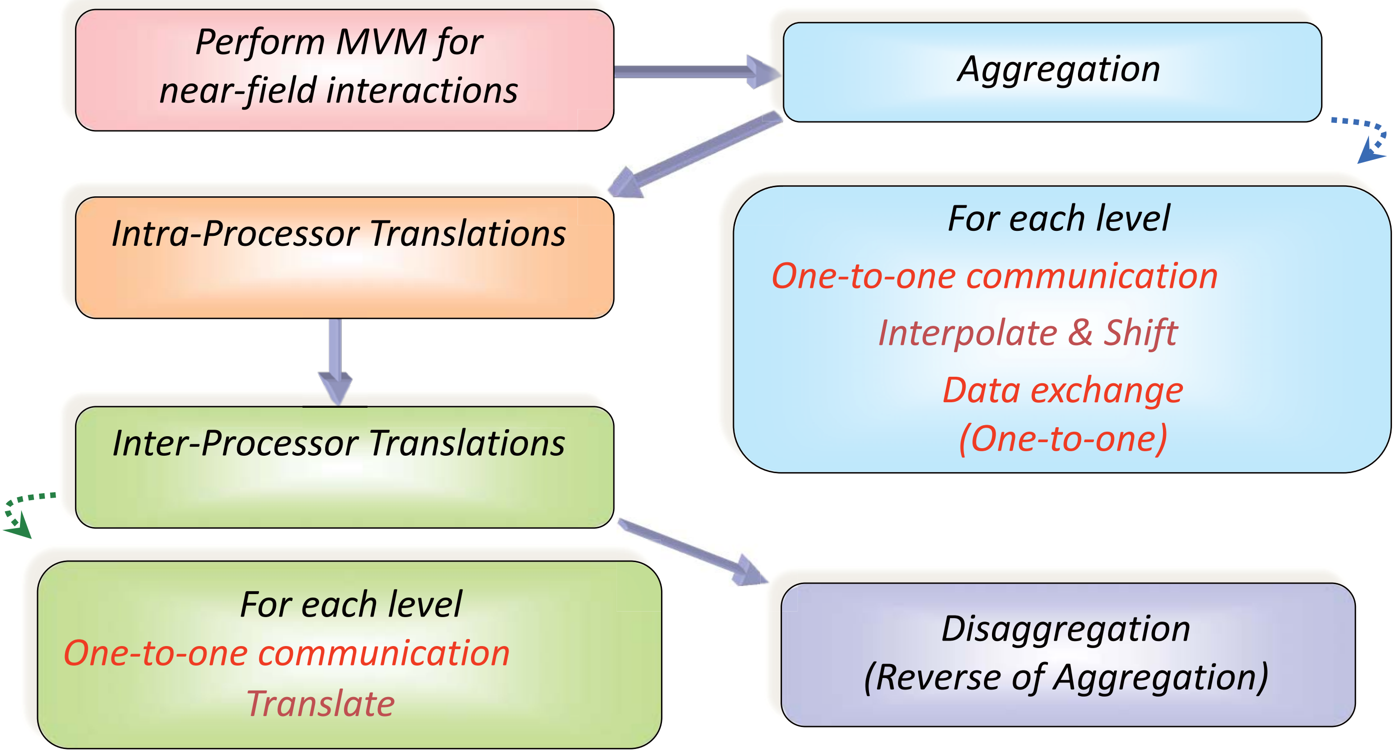
  - Among {1,3,5,7}
  - Among {2,4,6,8}

- *Processor pairing*



URSI AT-RASC

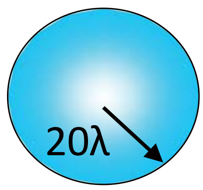
Matrix-Vector Multiplications



URSI AT-RASC

Advantages of the Hierarchical Strategy

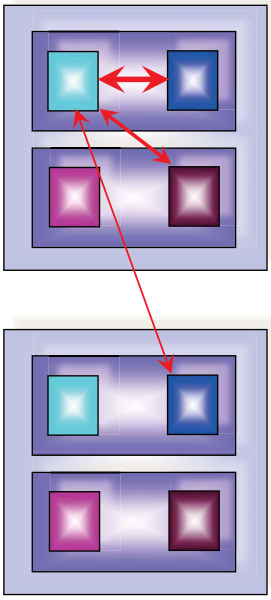
- *Improved load-balancing and reduced communications*
  - *The amount of communications is decreased*
  - *The number of communication events is reduced*

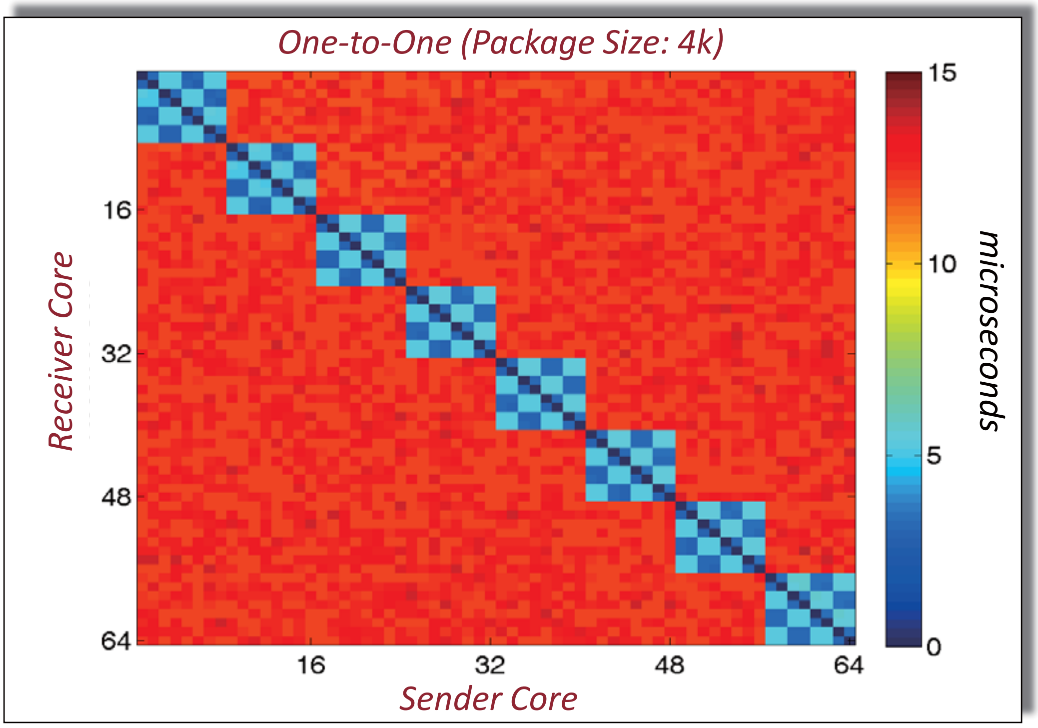


	HYBRID*		HIERARCHICAL	
	Events	Amount	Events	Amount
Interpolations	8320	1,676,352	2188	546,952
Data Exchanges	0	0	10	571,976
Switch	1160	171,680	0	0
Total Aggregation	9480	1,848,032	2198	1,118,928
Translation	6375	2,416,780	7215	2,003,928
TOTAL	15855	4,264,812	9413 (59%)	3,122,856 (73%)
Average Package Size	269 Bytes		332 Bytes (123%)	

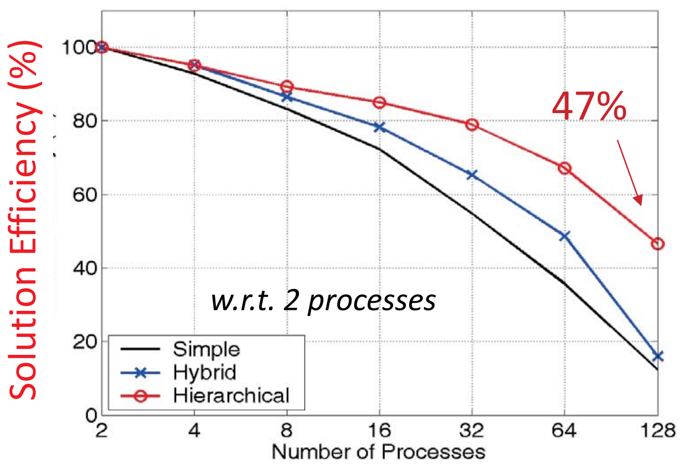
* S. Velamparambil and W. C. Chew, "Analysis and performance of a distributed memory multilevel fast multipole algorithm," *IEEE Trans. Antennas Propag.*, vol. 53, no. 8, pp. 2719-2727, Aug. 2005.

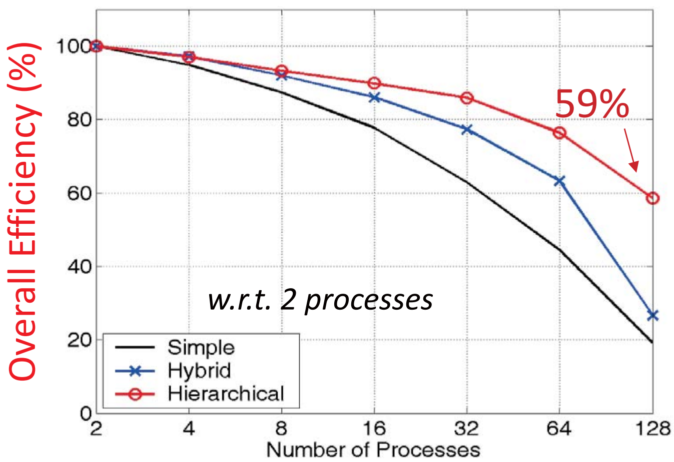
Parallel Computers

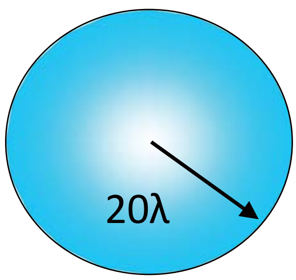




Results (Efficiency)







1,462,854 unknowns

System:

2.66 GHz Intel Xeon 5355 processors

Infiniband network

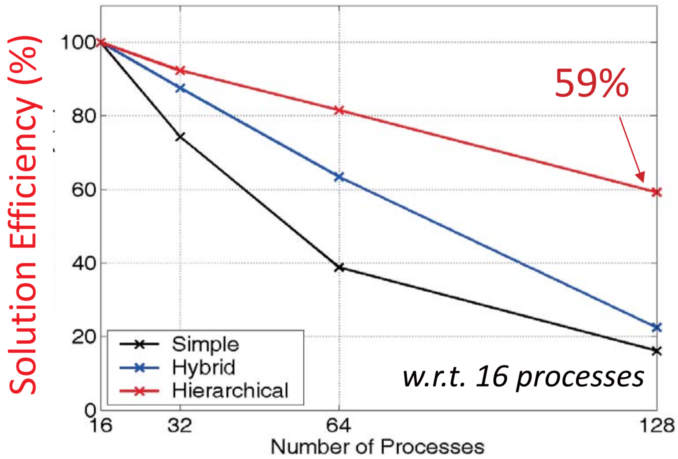
Parameters:

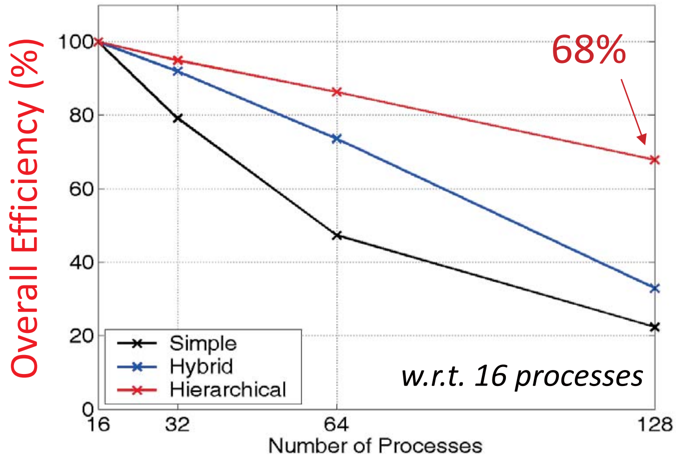
7-level MLFMA (Bottom-up clustering)

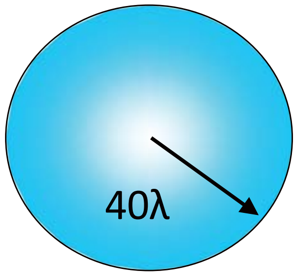
3-digits of accuracy

1e-6 residual error (27 iterations)

Results (Efficiency)



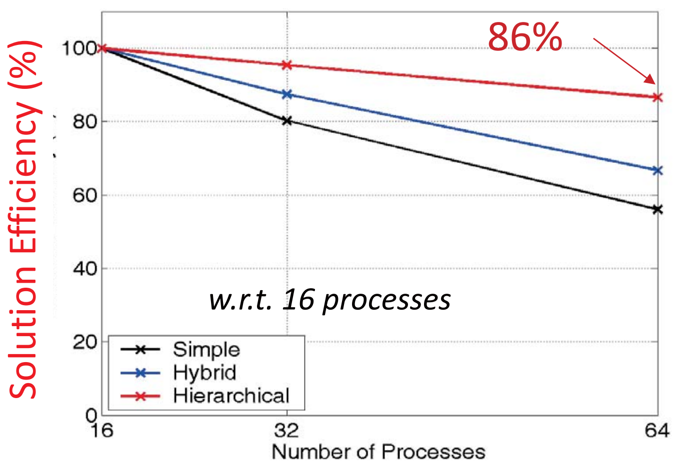


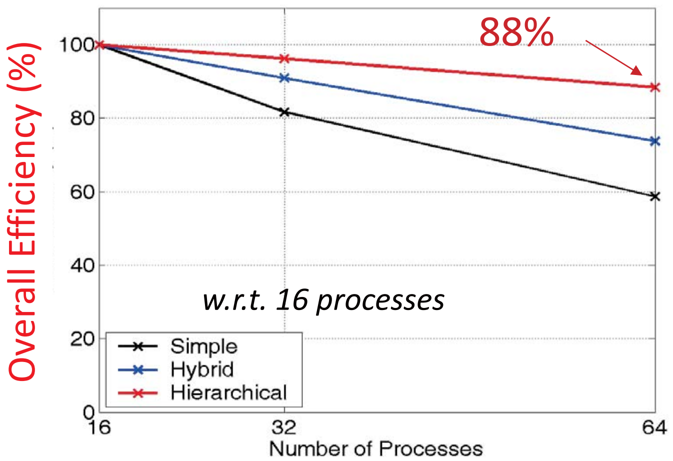


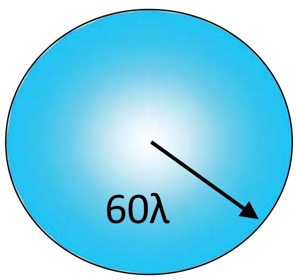
5,851,416 unknowns

System:
2.66 GHz Intel Xeon 5355 processors
Infiniband network
Parameters:
8-level MLFMA (Bottom-up clustering)
3-digits of accuracy
1e-6 residual error (30 iterations)

Results (Efficiency)





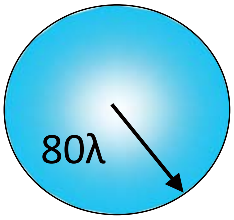


13,278,096 unknowns

System:
2.66 GHz Intel Xeon 5355 processors
Infiniband network
Parameters:
8-level MLFMA (Bottom-up clustering)
3-digits of accuracy
1e-6 residual error (43 iterations)

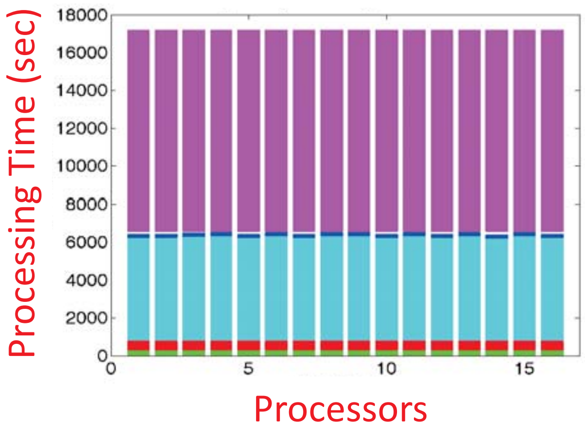
Results (Large Problems)

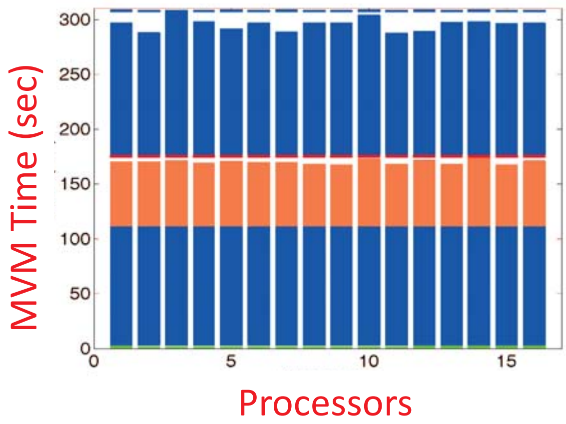
23,405,664 unknowns, 16 processors, BDP



Number of Levels	9
Smallest Box Size	0.156λ
Truncation Number	5 - 457
FMM Accuracy	2 digits
Residual	0.001

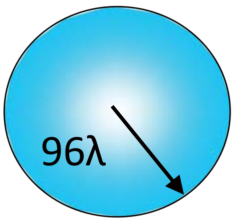
Setup Time	104 minutes
Solution Time	178 minutes
Iterations	17 BiCGStab
MVM Time	307 seconds
Total Memory	111 GB





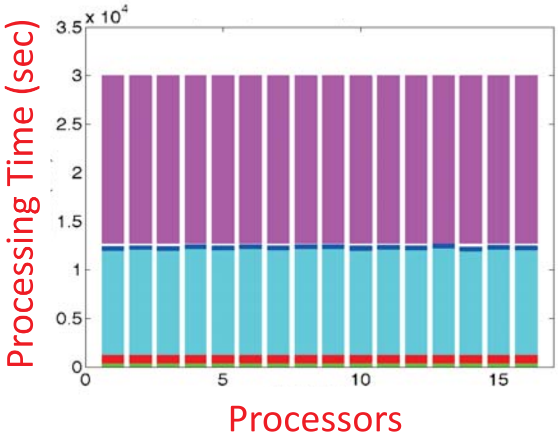
Results (Large Problems)

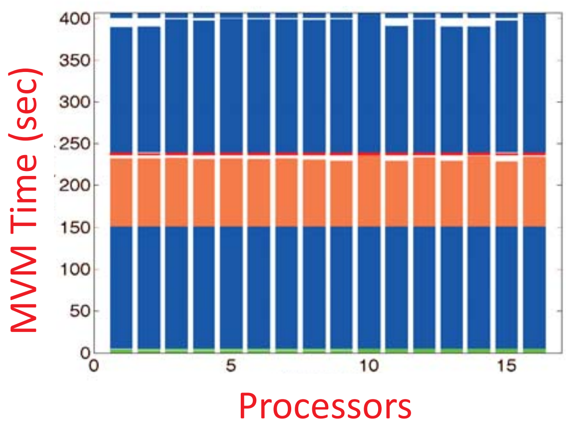
33,791,232 unknowns, 16 processors, BDP



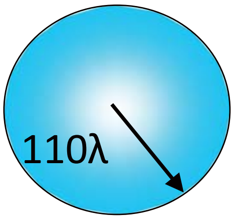
Number of Levels	9
Smallest Box Size	0.188λ
Truncation Number	6 - 546
FMM Accuracy	2 digits
Residual	0.001

Setup Time	205 minutes
Solution Time	289 minutes
Iterations	21 BiCGStab
MVM Time	406 seconds
Total Memory	179 GB





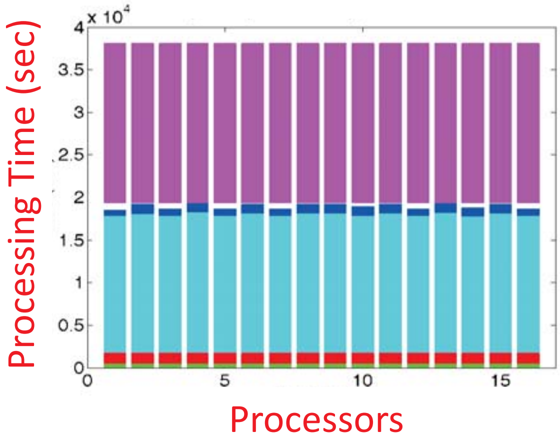
Results (Large Problems)

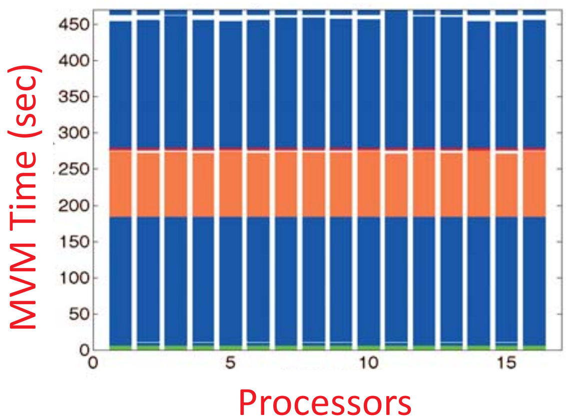


41,883,648 unknowns, 16 processors, BDP

Number of Levels	9
Smallest Box Size	0.215λ
Truncation Number	6 - 623
FMM Accuracy	2 digits
Residual	0.001

Setup Time	313 minutes
Solution Time	314 minutes
Iterations	19 BiCGStab
MVM Time	467 seconds
Total Memory	223 GB



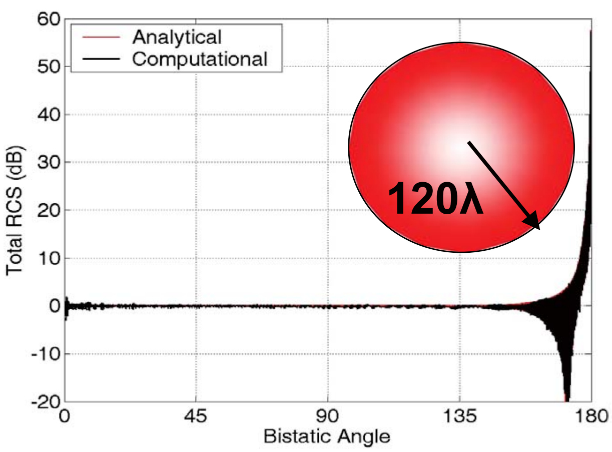


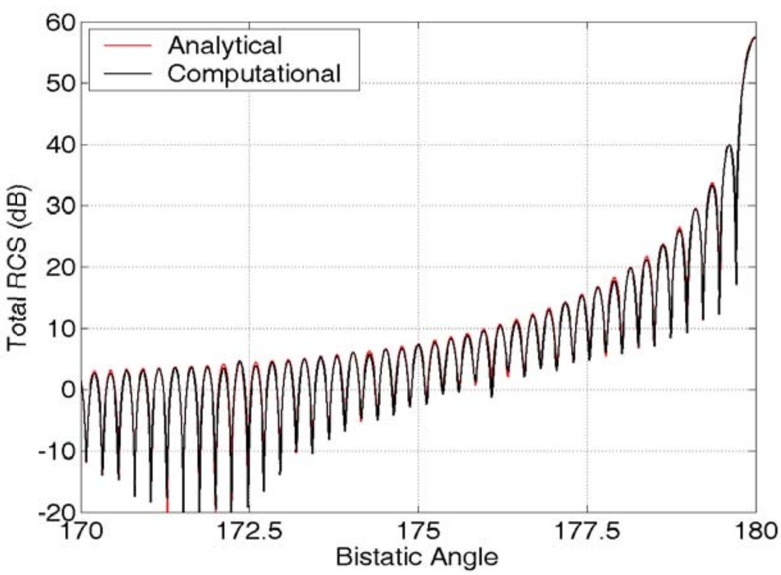
53 Million Unknowns

Sphere with radius of 120λ and diameter of 240λ

November 2007

53,112,384 Unknowns





Intel Pamphlet on the World Record

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,

BiLCEM

Available at www.abakus.computing.technology

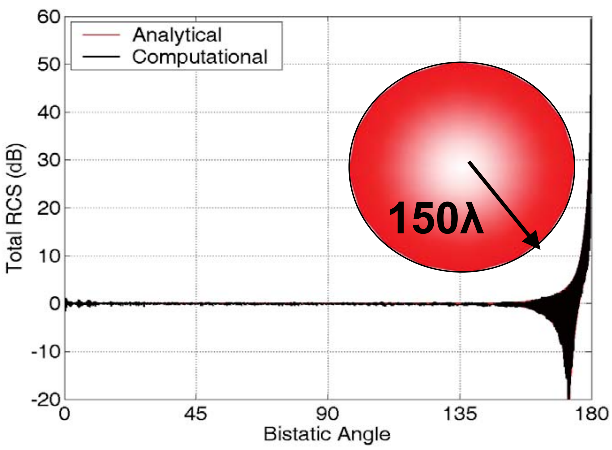
85 Million Unknowns

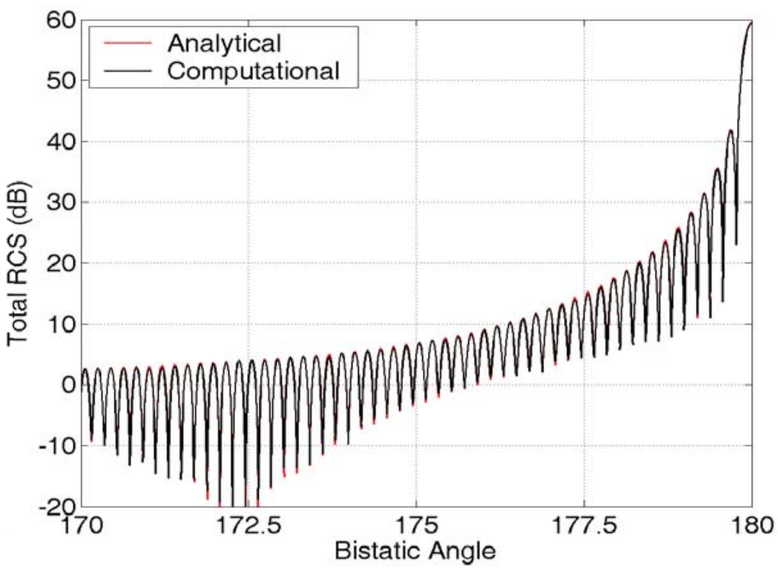
January 2008

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





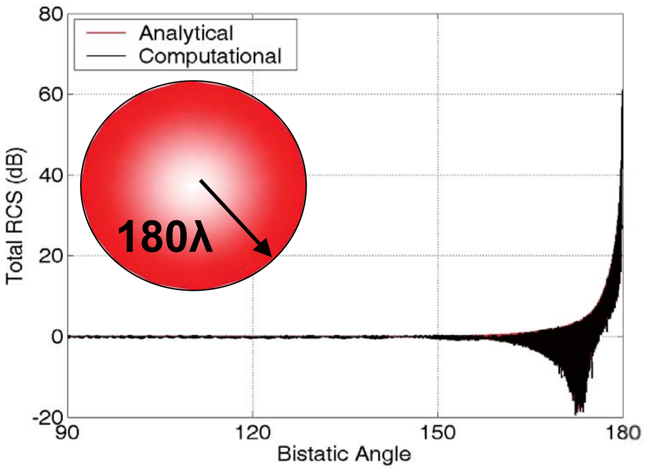
135 Million Unknowns

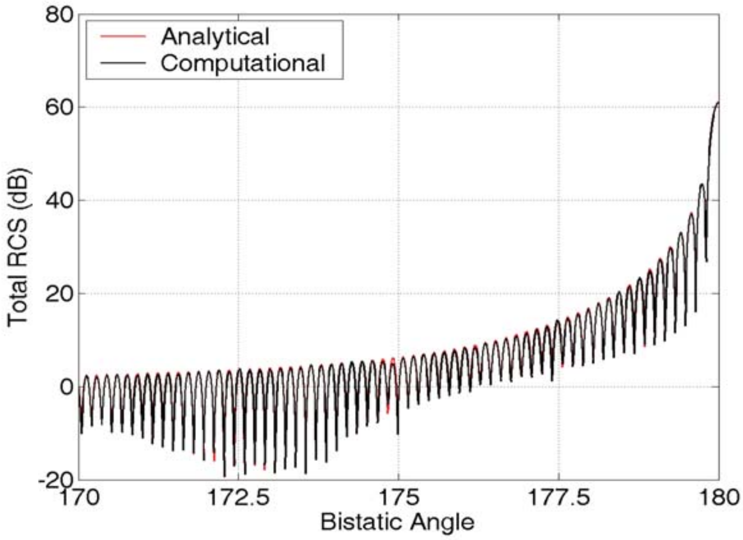
August 2008

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





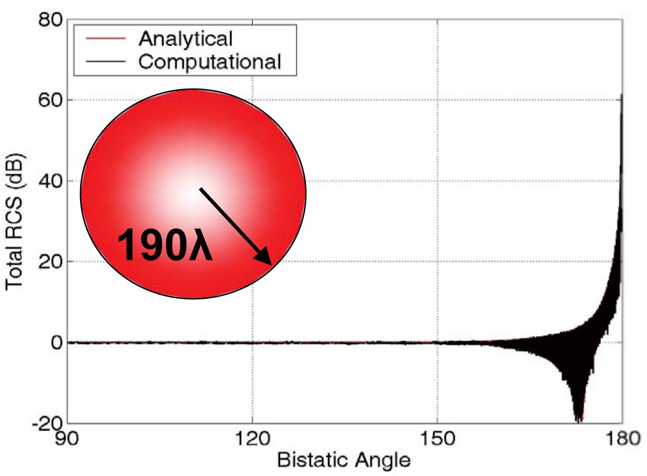
167 Million Unknowns

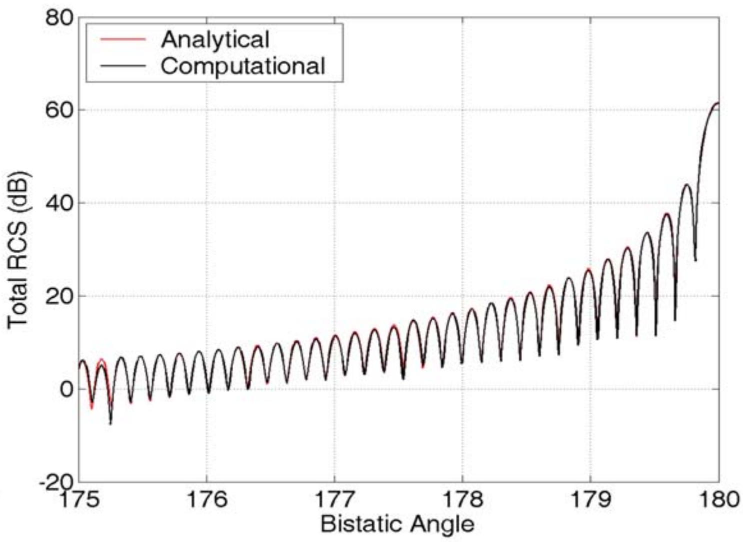
August 2008

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





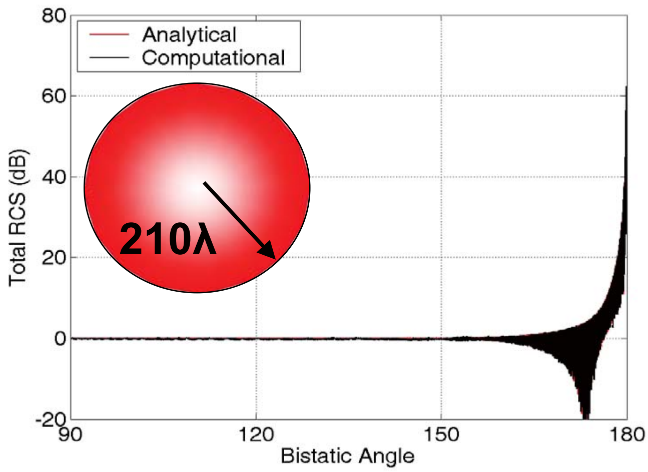
205 Million Unknowns

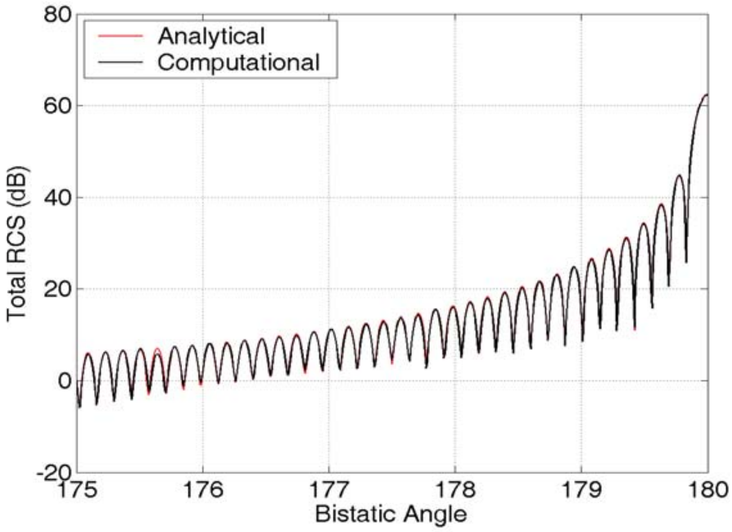
September 2008

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





Prof. Levent Gürel — ABAKÜS — http://abakus.computing.technology/

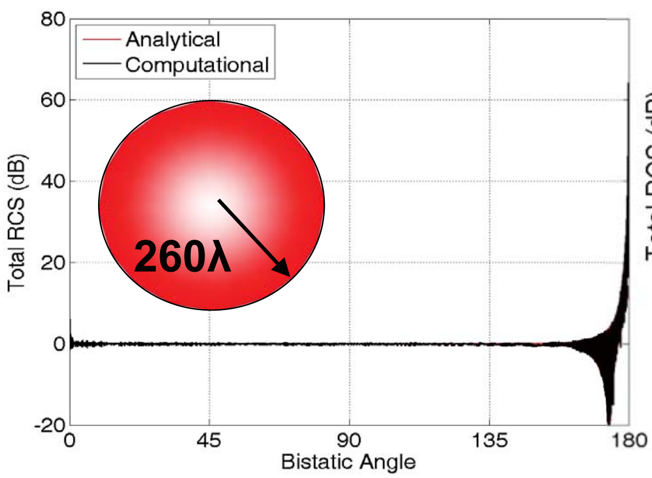
307 Million Unknowns

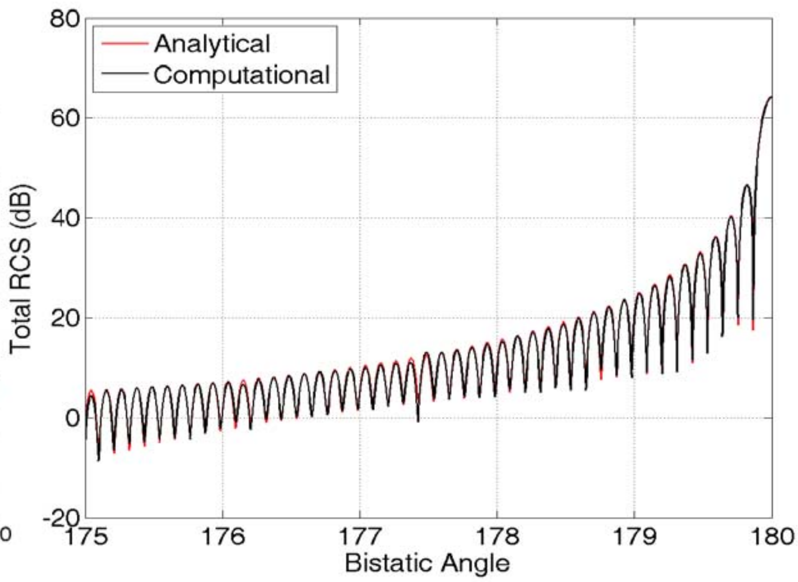
December 2009

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





Prof. Levent Gürel — ABAKÜS — http://abakus.computing.technology/

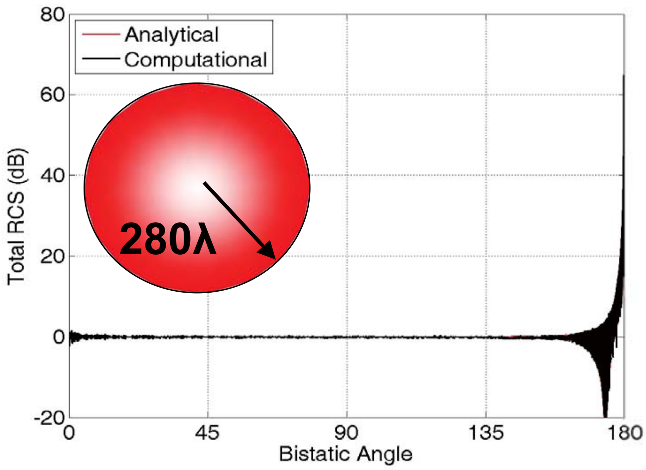
375 Million Unknowns

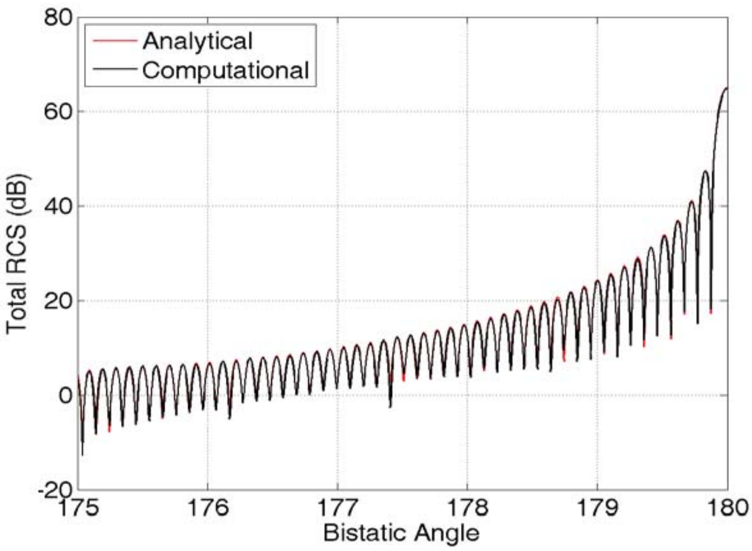
December 2009

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





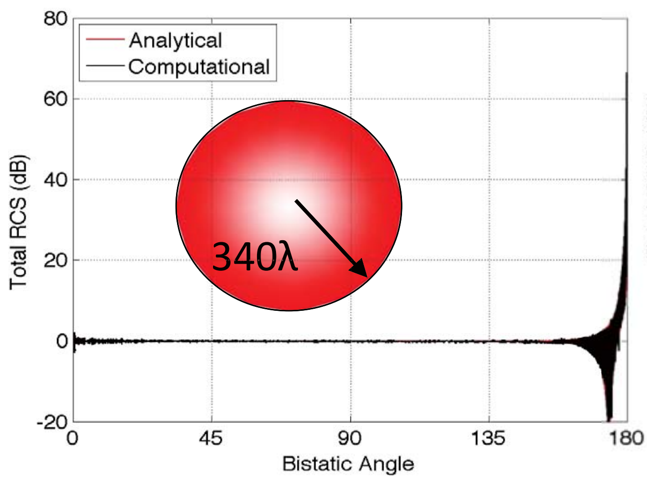
540 Million Unknowns

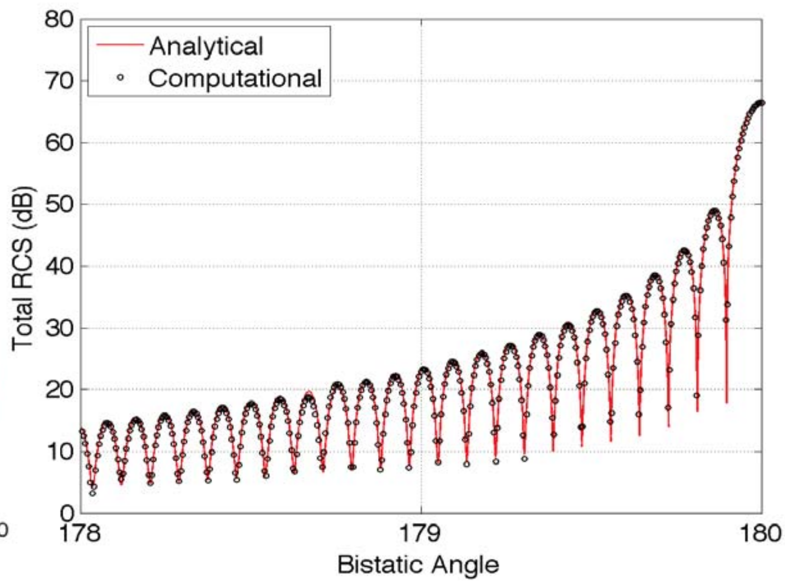
September 2010

Sphere with radius of 340λ and diameter of 680λ

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

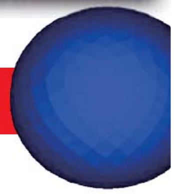
540,659,712 Unknowns





670 Million Unknowns

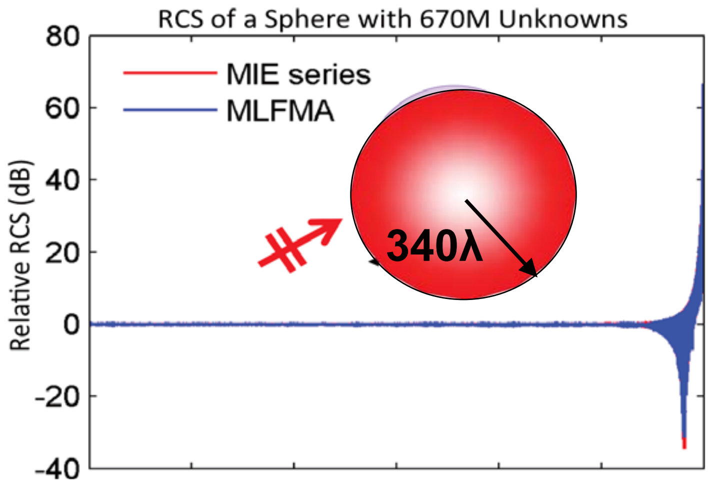
2013

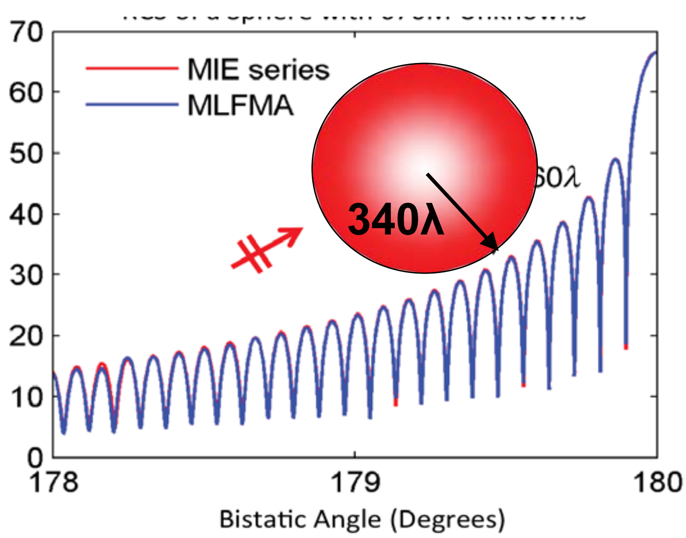


Sphere with radius of 340λ and diameter of 680λ

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

670 Million Unknowns



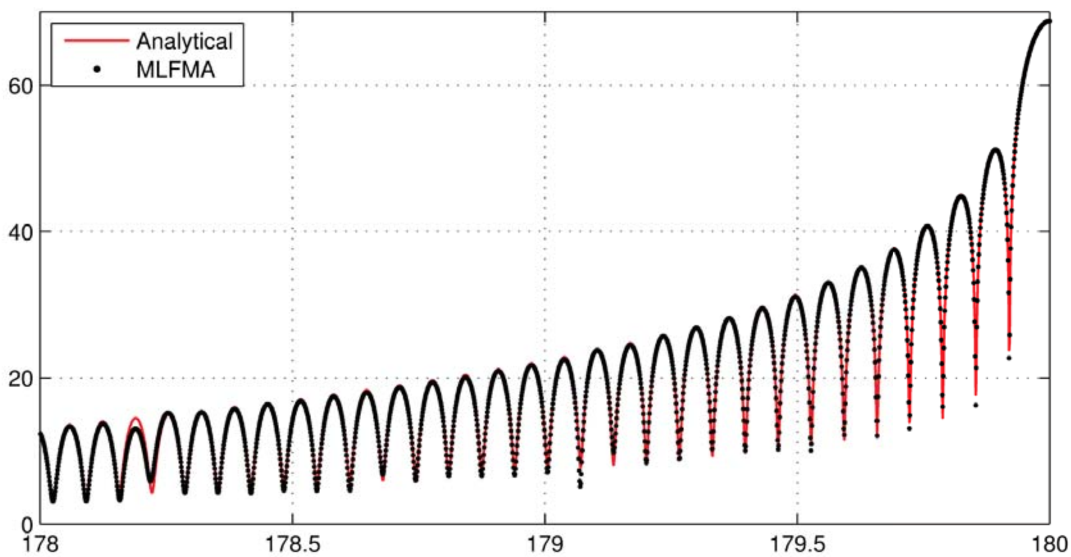


850 Million Unknowns

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.



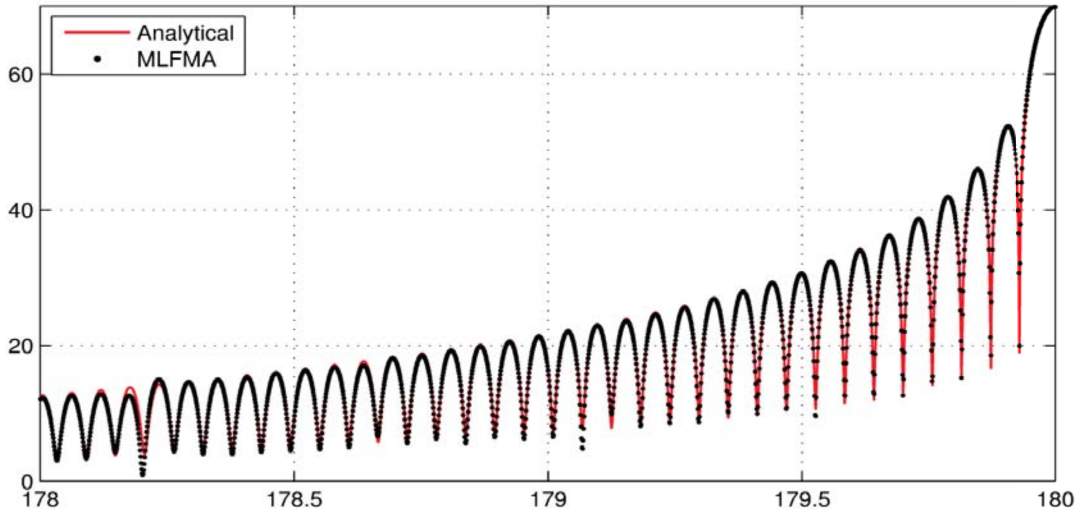
1.1 Billion Unknowns

2014

Sphere with radius of 500λ and diameter of 1000λ

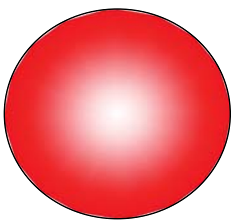
Scattering results are compared to analytical values to demonstrate the accuracy of the numerical solution.

1000λ



BENCHMARKING

Available from
www.abakus.computing.technology



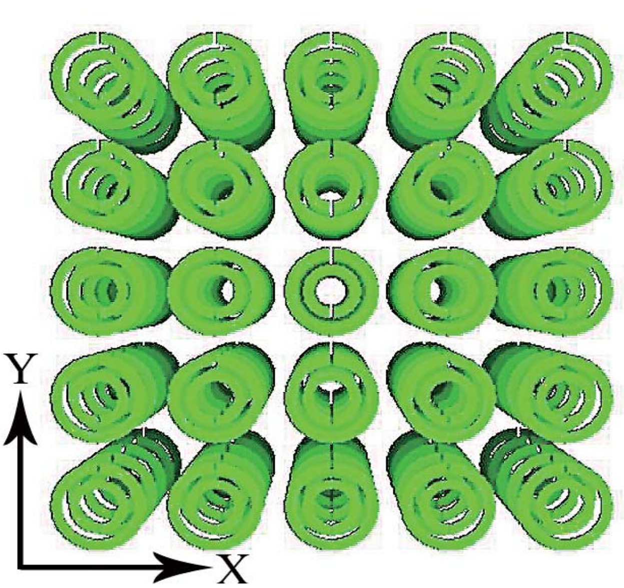
Scattering from sphere (radius: 20λ - 340λ)
Web-based application: Upload the computational results and get the error with respect to analytical Mie-series solutions.

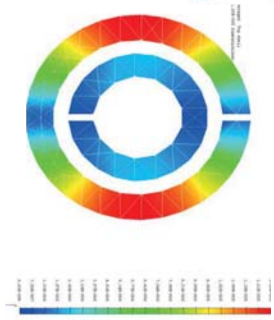
Scattering from NASA Almond (size: 94λ - 1514λ)
Web-based application: Upload the computational results and get the error with respect to our results.

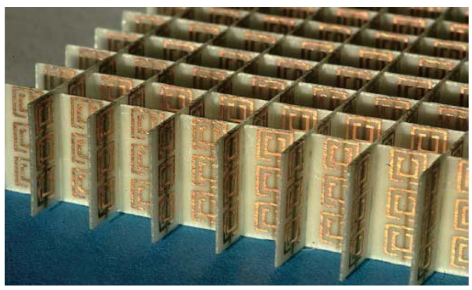
WEB-BASED BENCHMARKING TOOL

Metamaterials

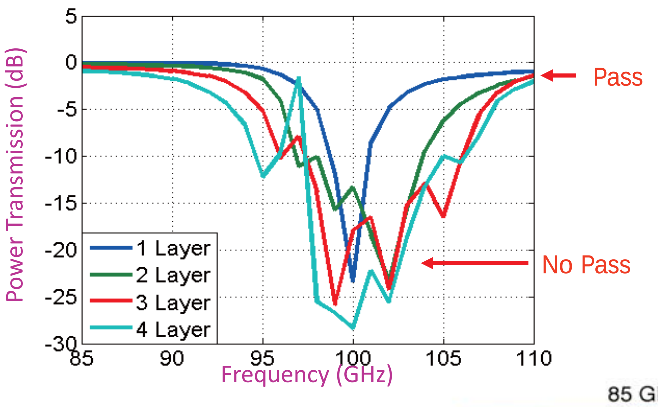
Split-Ring Resonators

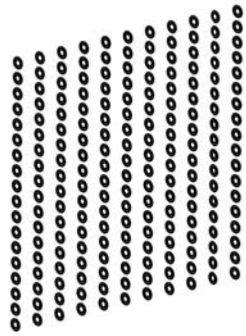


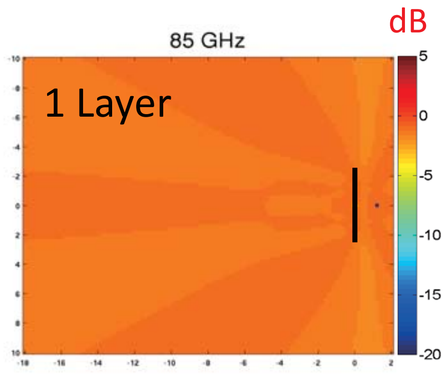


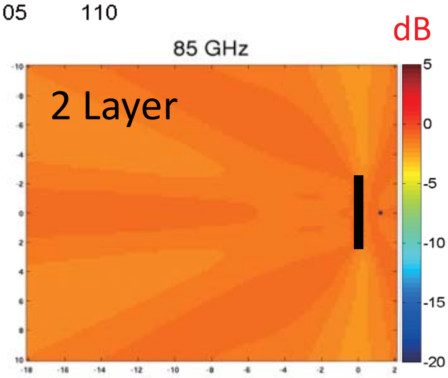


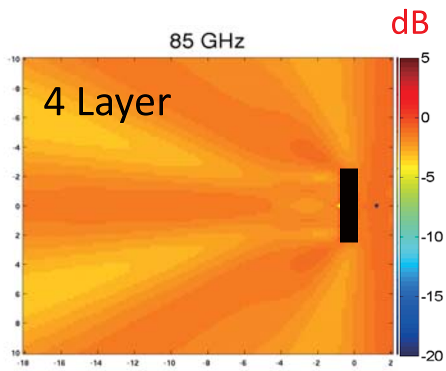
SRR Walls







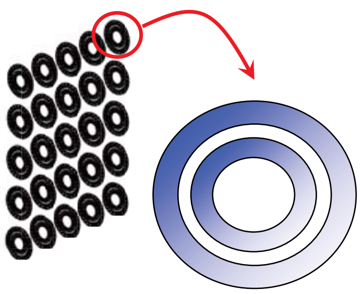




Meta Property:
Stop band in frequency!

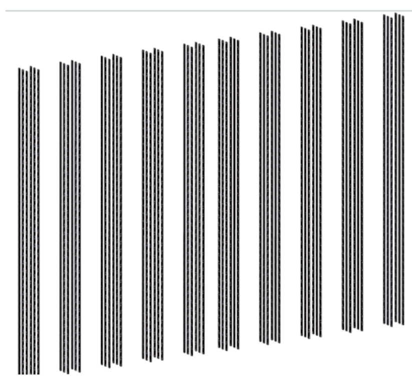
Special Configurations

Closed-Ring Resonators (CRRs)



All pass!

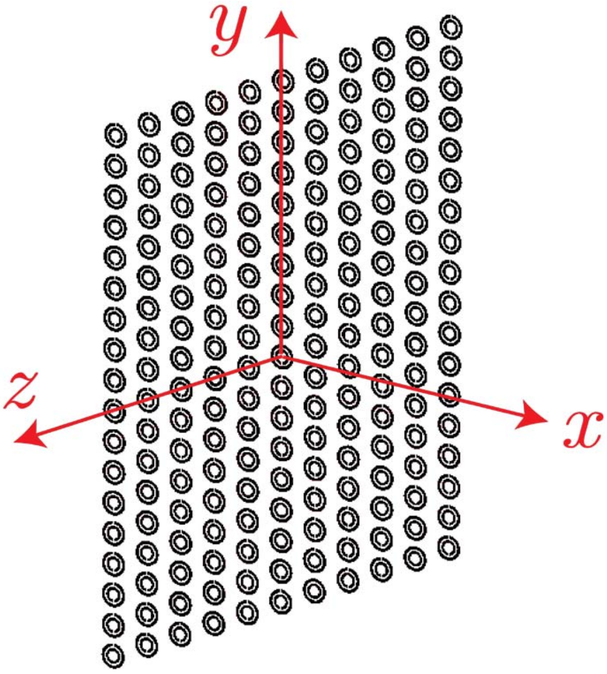
Thin Wire Array (TWA)



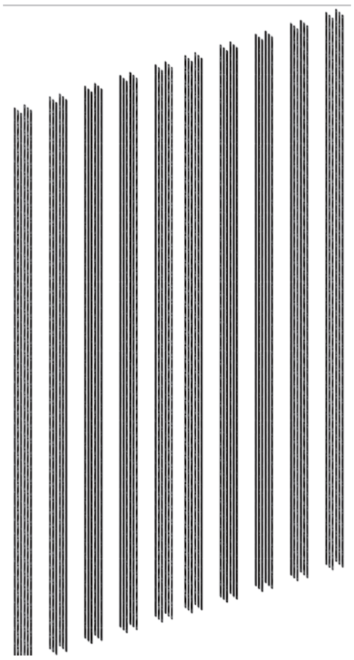
No pass!

Composite Metamaterial (CMM)

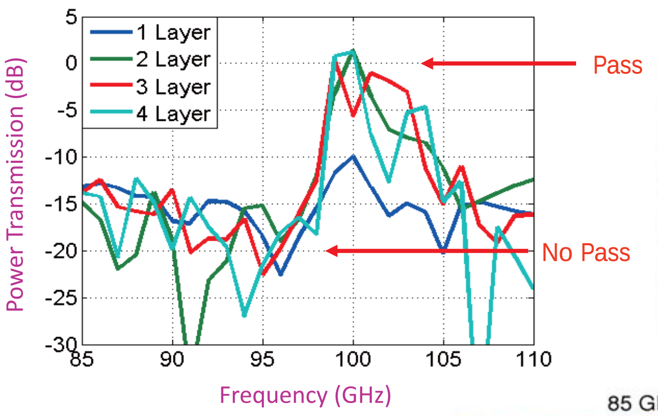
Split-Ring Resonators (SRRs)

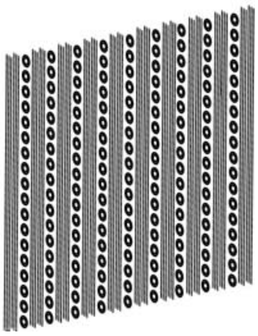


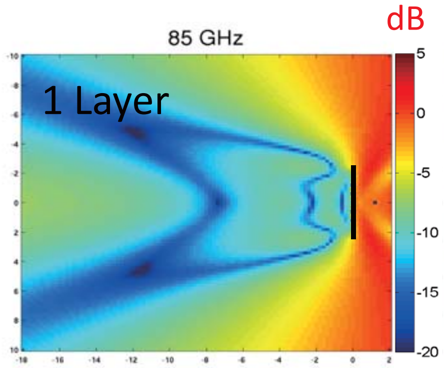
Thin Wire Array (TWA)

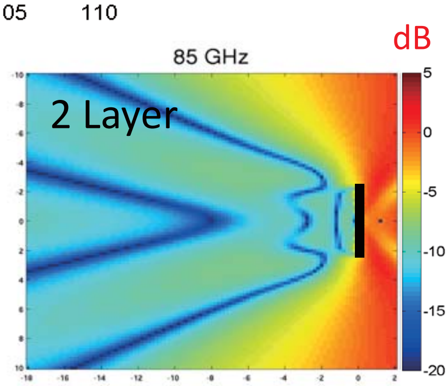


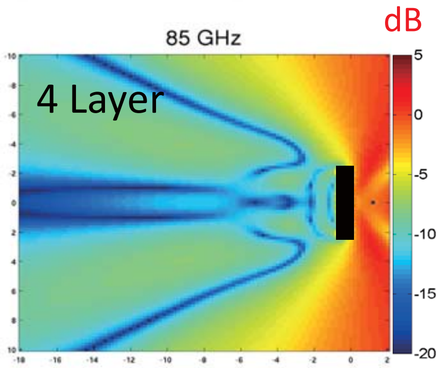
CMM Walls







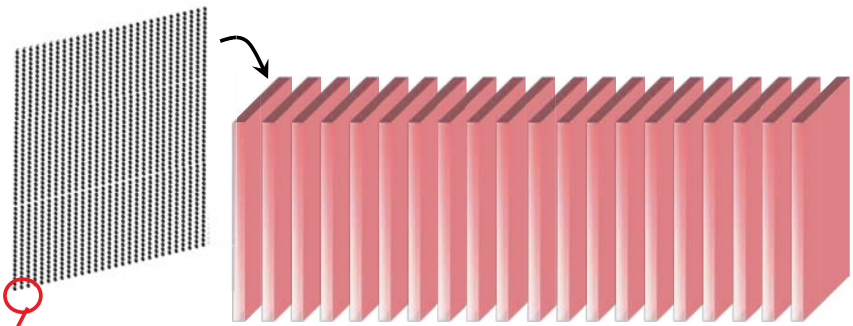


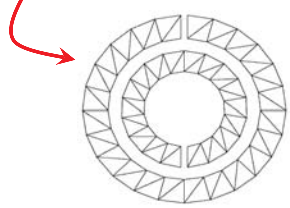


Meta Property:
Pass band in
frequency!

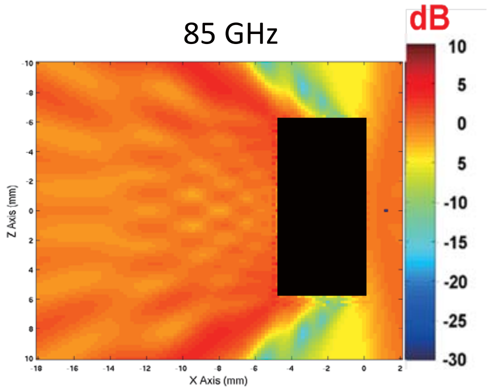
Large MM Problem

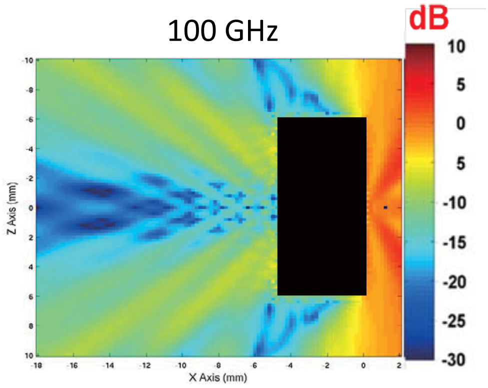
20 x 51 x 29 SRR Block





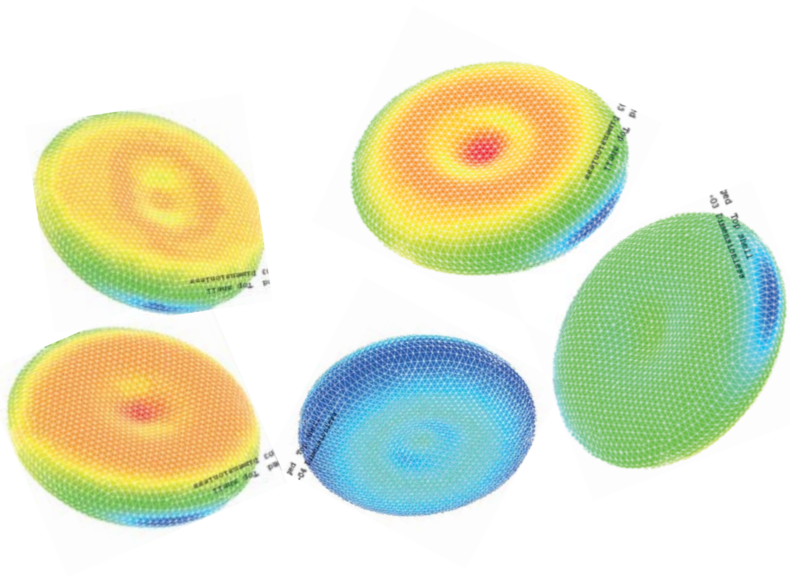
2,425,560 Unknowns
9381 Seconds

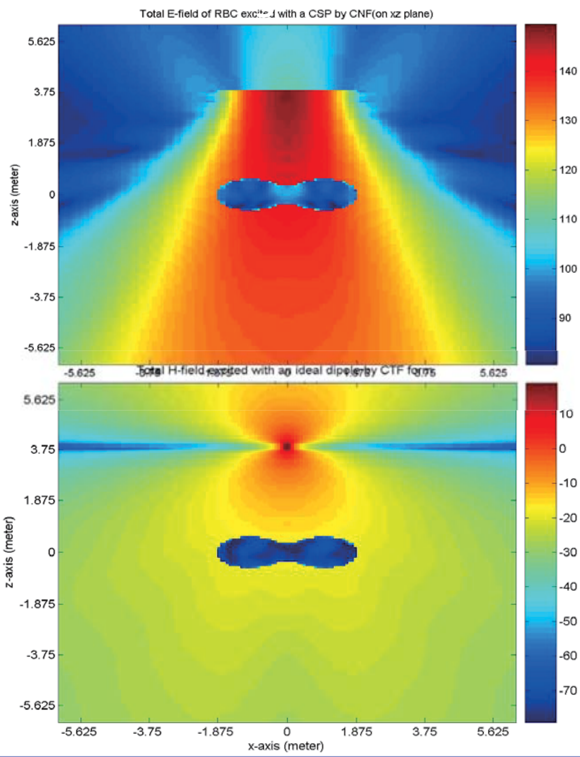




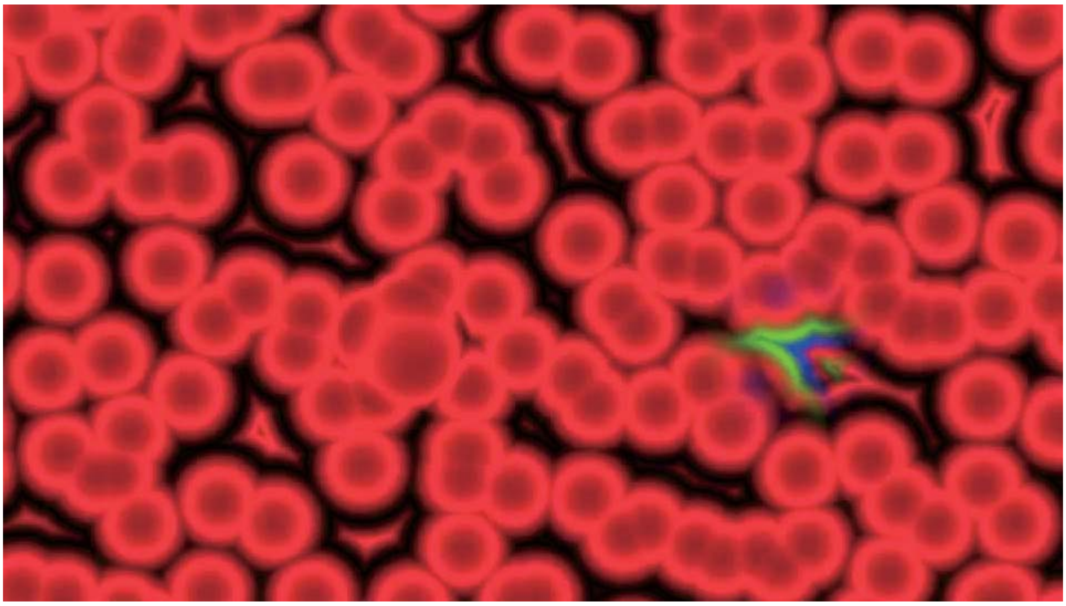
MLFMA parallelized into 64 process on a cluster of Intel-Xeon processors connected via Infiniband network

Scattering from and Imaging of Red Blood Cells

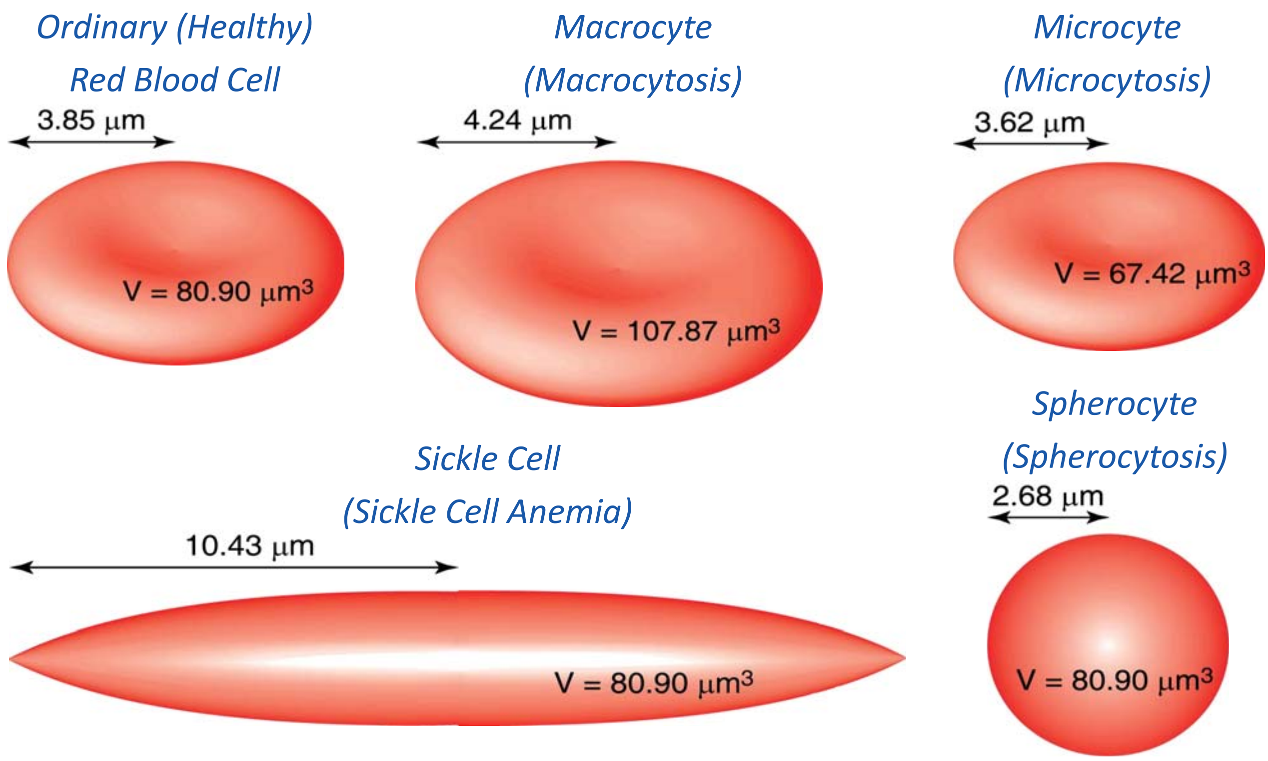




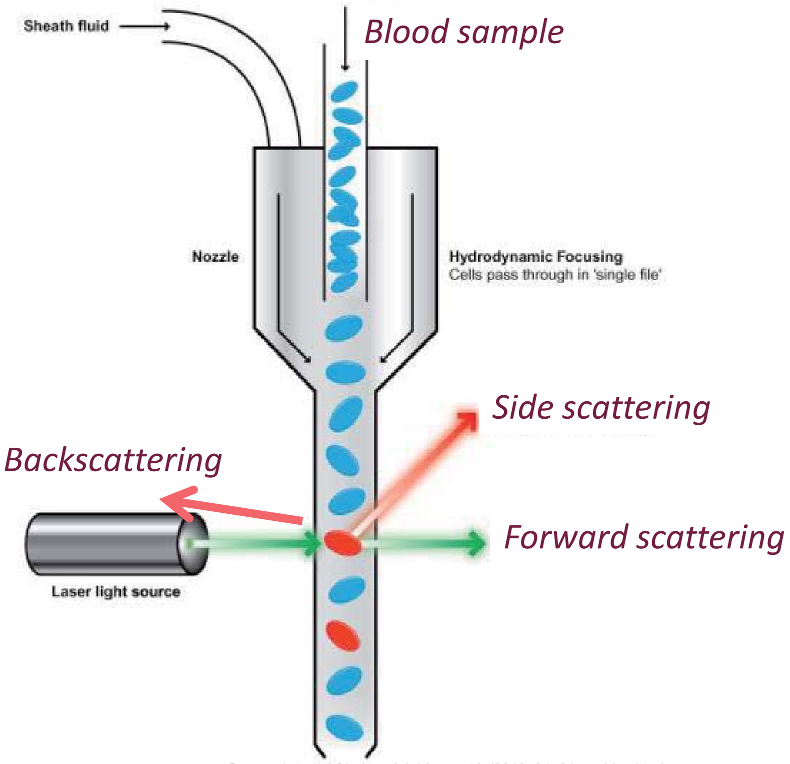
Red Blood Cells (RBCs)



Red Blood Cells (RBCs)

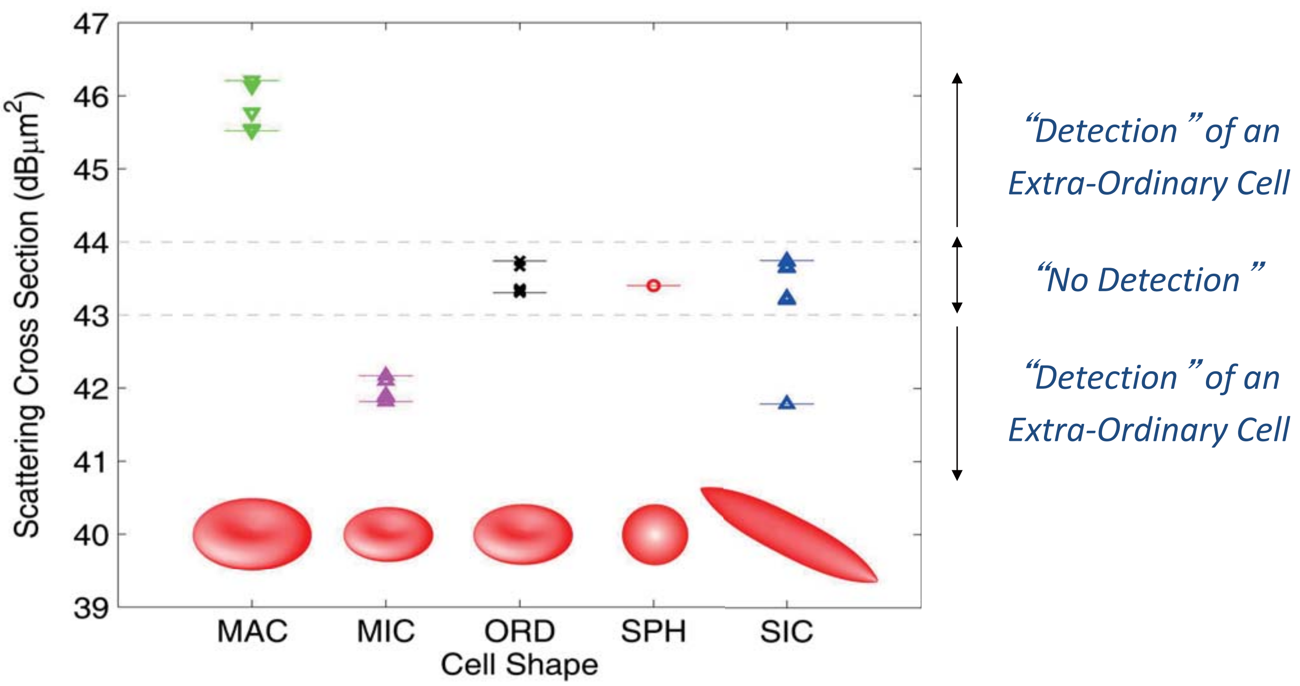


Flow Cytometry



Source: http://nirfriedmanlab.blogspot.in/2010_04_01_archive.html

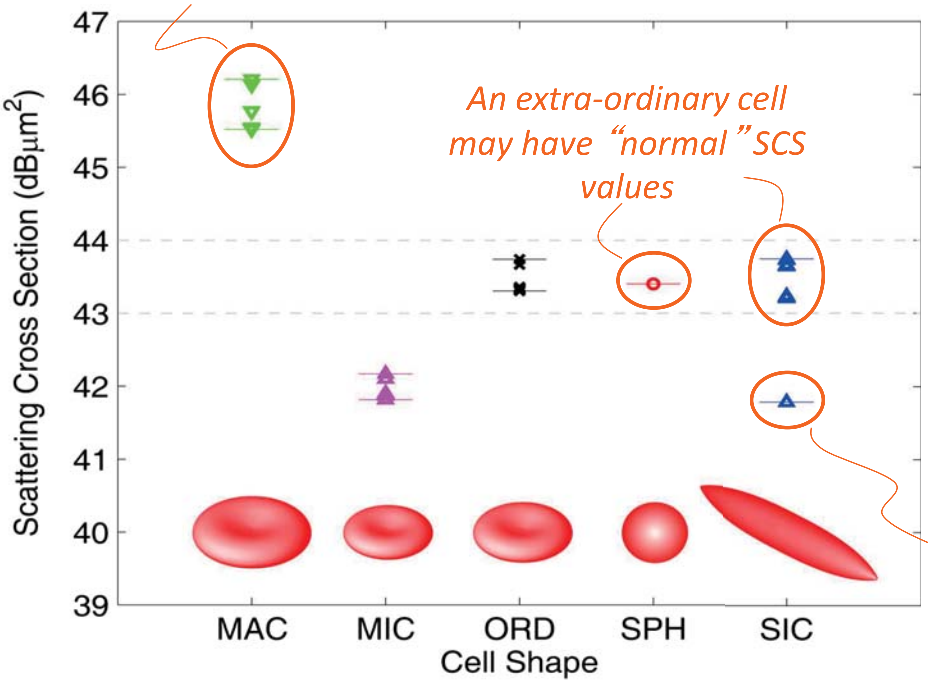
Forward Scattering



URSI AT-RASC

Forward Scattering

An extra-ordinary cell can be detected for all orientations



"Detection" of an Extra-Ordinary Cell

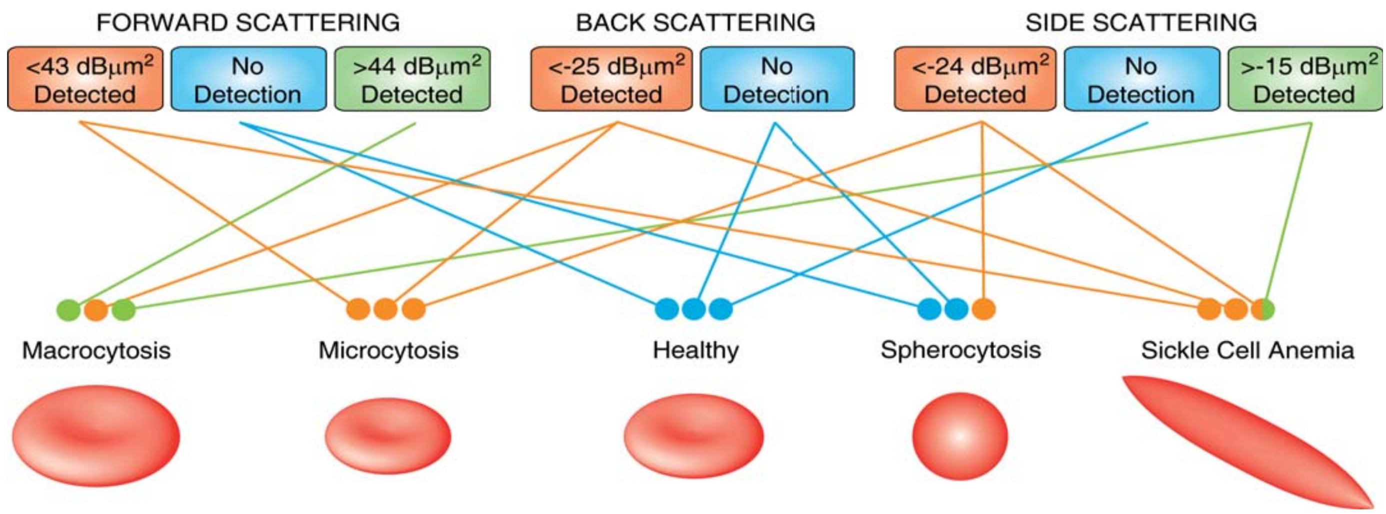
"No Detection"

"Detection" of an Extra-Ordinary Cell

An extra-ordinary cell can be detected for some orientations

URSI AT-RASC

Decision Chart



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