SIAM Conference on Computational Science and Engineering

MS27:

Featured Minisymposium:

Fast Multipole Methods Maturing at 30 Years

Prof. Lorena A. Barba

Mechanical and Aerospace Engineering

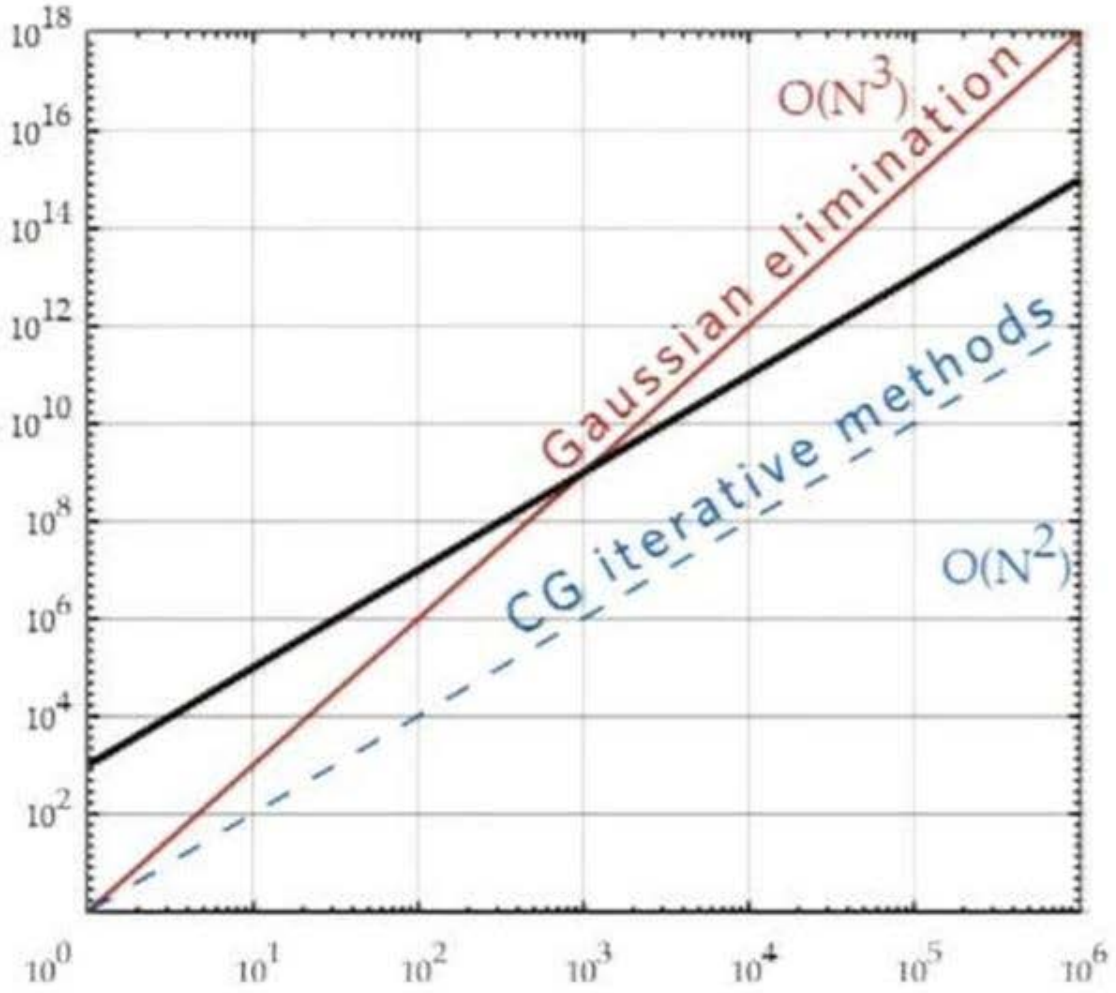
The George Washington University

Twitter: @LorenaABarba


“Complexity trumps hardware.”

The story of the conjugate gradient method

- CG iterations bring the $O(N^3)$ cost to $O(N^2)$
- 1950s — N too small for CG to be competitive
- 1970s — becomes popular



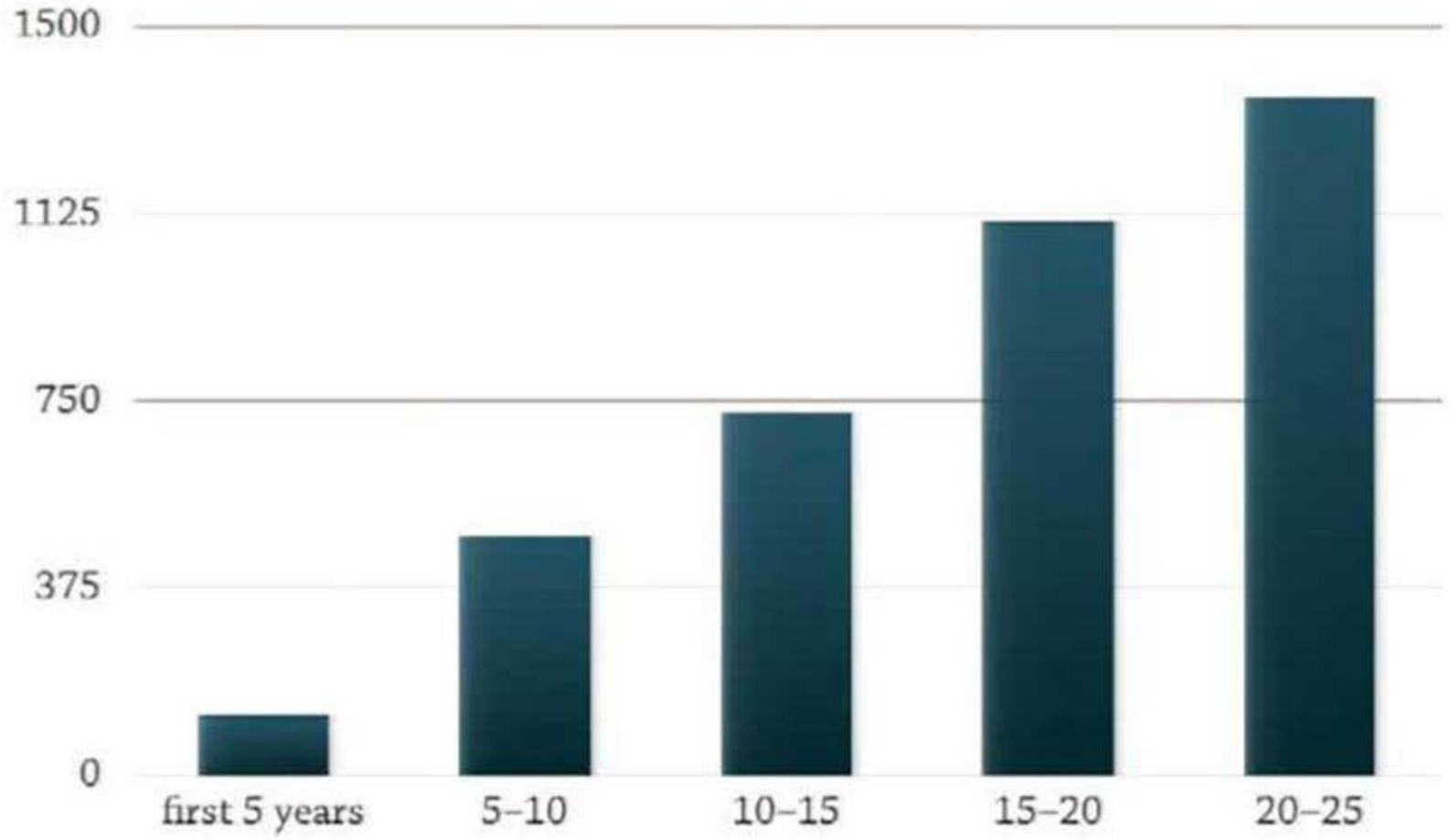
Google "a fast algorithm for particle simulations"

Scholar About 2,140 results (0.11 sec)

A fast algorithm for particle simulations
L Greengard, V Rokhlin - Journal of computational physics, 1987 - Elsevier
Abstract An algorithm is presented for the rapid evaluation of the potential and force fields in systems involving large numbers of particles whose interactions are Coulombic or gravitational in nature. For a system of N particles, an amount of work of the order O (N 2) ...
Cited by 3874 Related articles All 27 versions Import into BibTeX Saved More

A fast algorithm for particle simulations
L Greengard, V Rokhlin - Journal of Computational Physics, 1997 - Elsevier
An algorithm is presented for the rapid evaluation of the potential and force fields in systems involving large numbers of particles whose interactions are Coulombic or gravitational in nature. For a system ofNparticles, an amount of work of the orderO (N2) has traditionally ...
Cited by 196 Related articles All 15 versions Import into BibTeX Save More

Number of citations in the years after the publication of Greengard & Rocklin, 1987



SIAM Conference on Computational Science and Engineering

Figure courtesy Thomas A. Brunner and Tzanio V. Kolev, SISC, Vol.33, 5-6

February 25-March 1, 2013

The Westin Boston Waterfront

Boston, Massachusetts, USA

SIAM CSE 13

- **MS11**—Fast Algorithms for Integral Equations Methods and Their Applications
  - *Organizer*: Prabir Daripa
- **MS31**—Fast Algorithms in Potential Theory (2 Parts)
  - *Organizers*: Bryan D. Quaife, George Biros
- **MS72**—Integral Equation Methods in Complex Geometry (3 Parts)
  - *Organizers*: Leslie Greengard, Andreas Kloeckner
- **MS132**—Applications and New Developments in Fast-multipole and Tree-based Methods (2 Parts)
  - *Organizer*: Lorena A. Barba, Rio Yokota, Cris R. Cecka

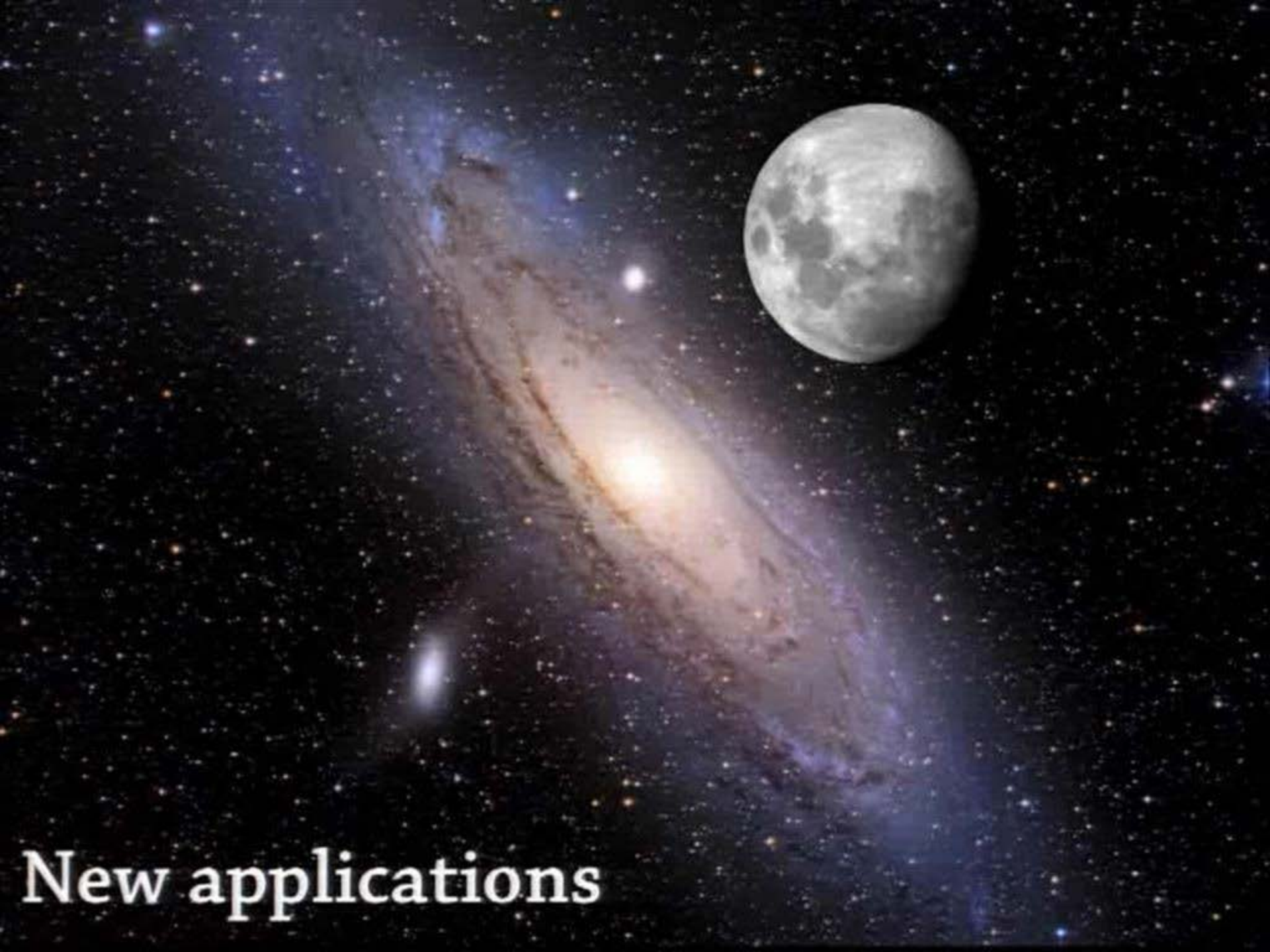
Lloyd Trefethen, 1998:

Predictions for Scientific Computing 50 Years From Now

#7

"Multipole methods and their descendants will be ubiquitous."

—L. N. Trefethen, 1998

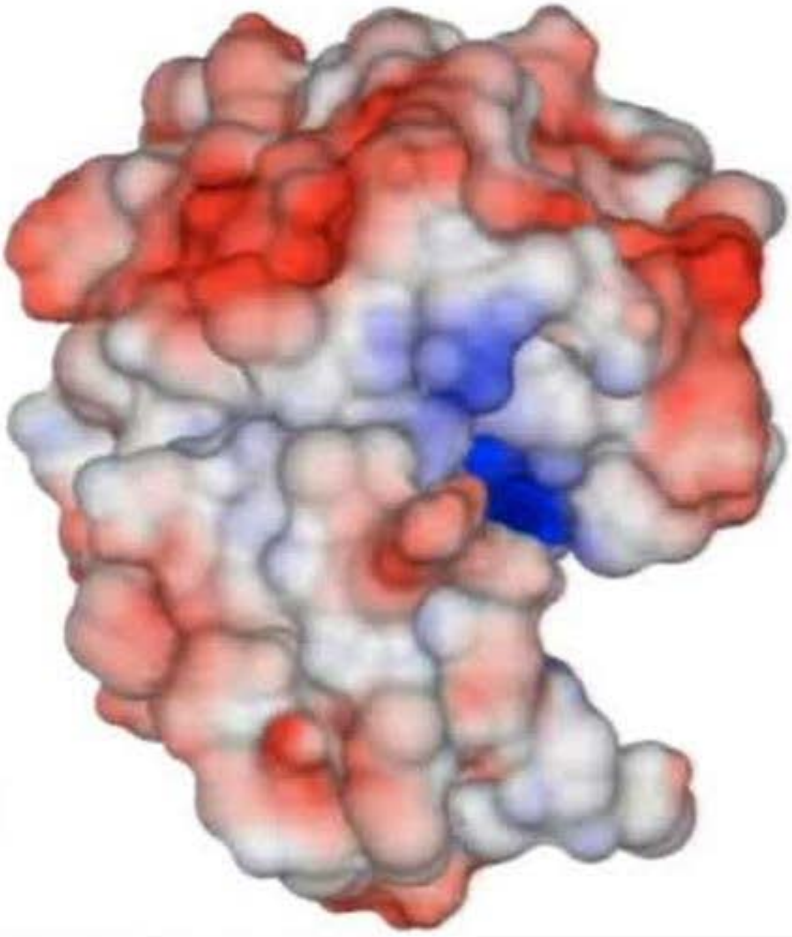

New applications

A biomolecular electrostatics solver using Python, GPUs and boundary elements that can handle solvent-filled cavities and Stern layers

Christopher D. Cooper [a], Jaydeep P. Bardhan [b], L.A. Barba [a,*,1]

[a] Mechanical Engineering, Boston University, Boston, MA 02215, USA

[b] Electrical and Computer Engineering, Northeastern University, Boston, MA 02115, USA

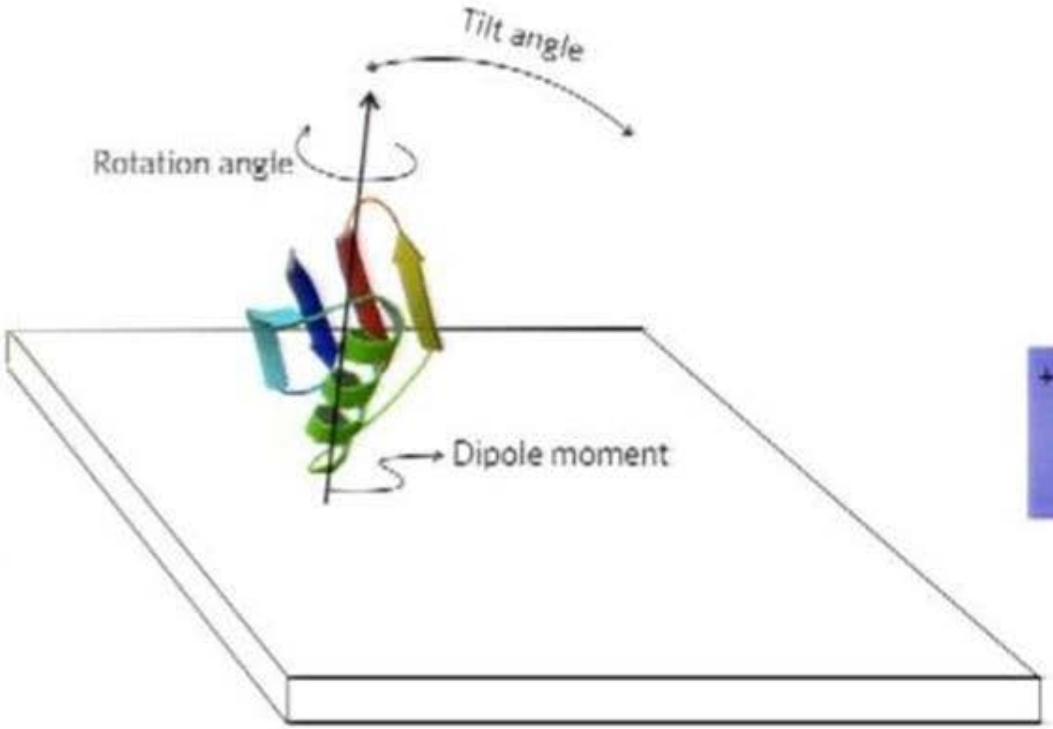


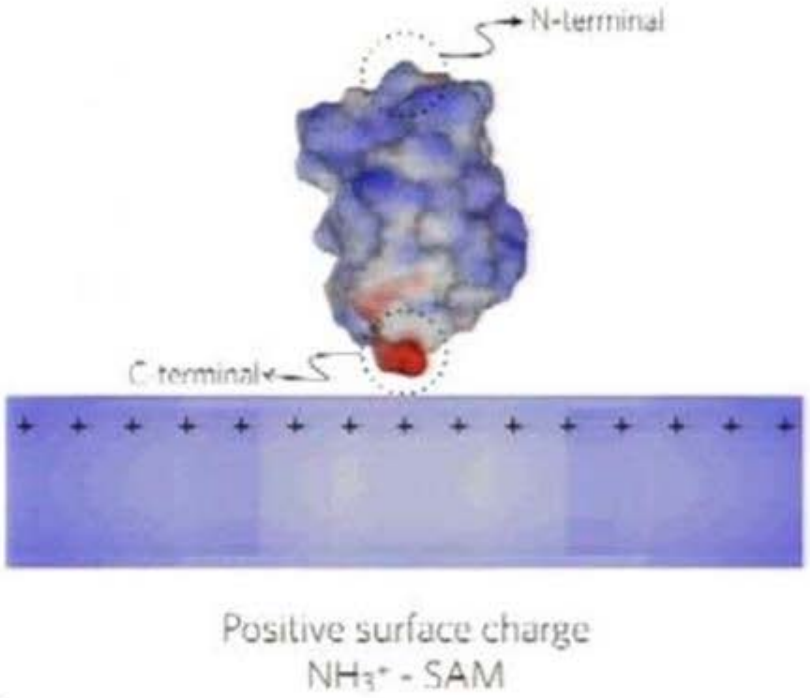
https://github.com/barbagroup/pygbe

Preprint:

Probing protein orientation near charged surfaces with an implicit-solvent model and the PyGBe code

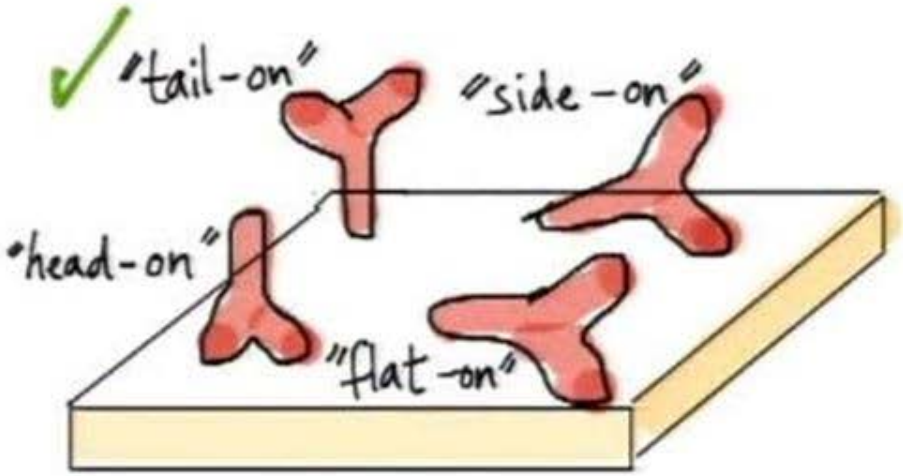
Christopher D. Cooper[1, a)] and Lorena A. Barba[2, b)]

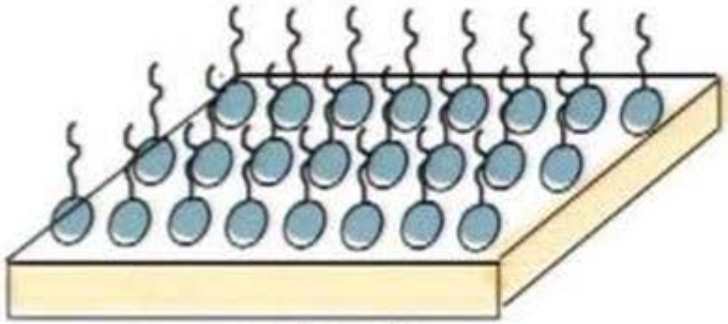




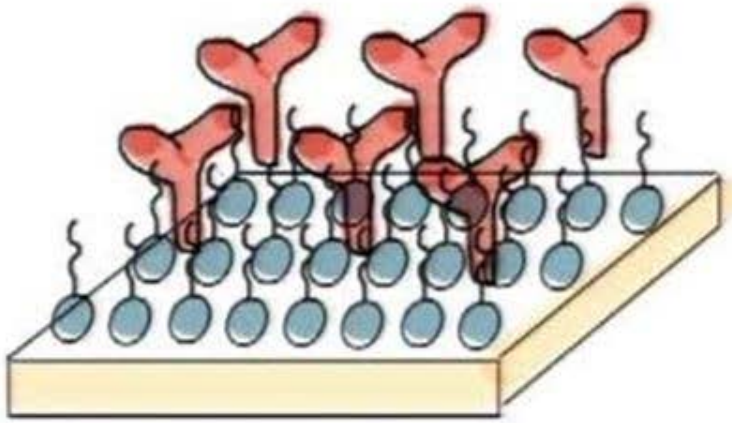
Positive surface charge
NH_3^+ - SAM

Antibody-based sensors





Self-assembled Monolayer on a gold electrode.

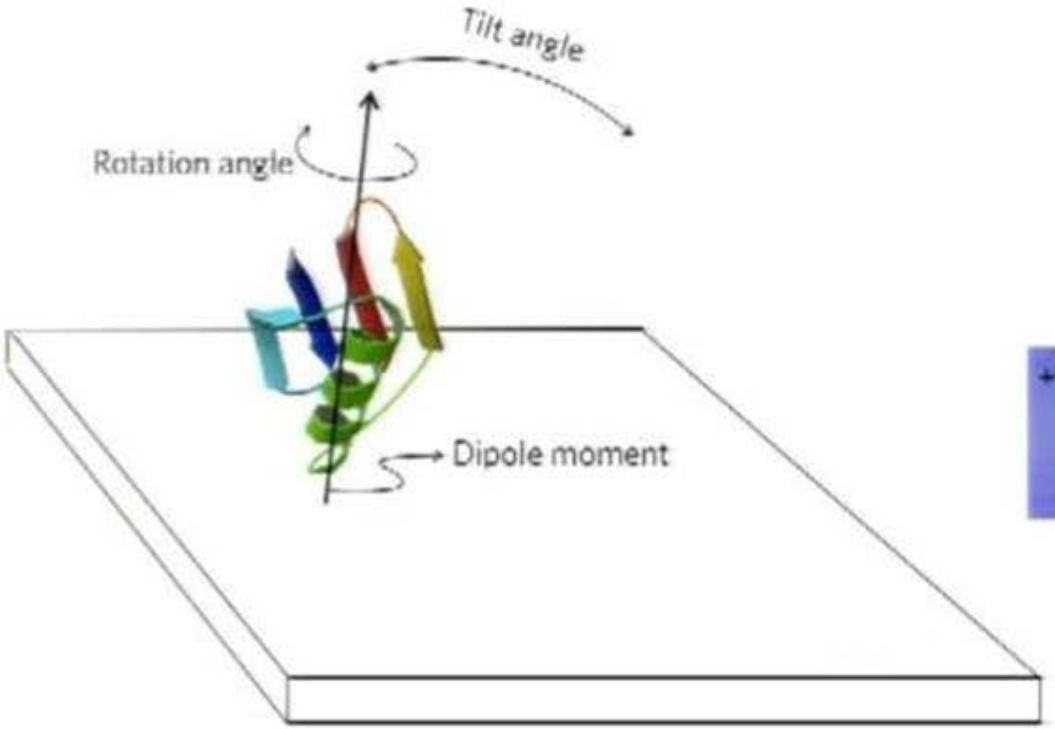


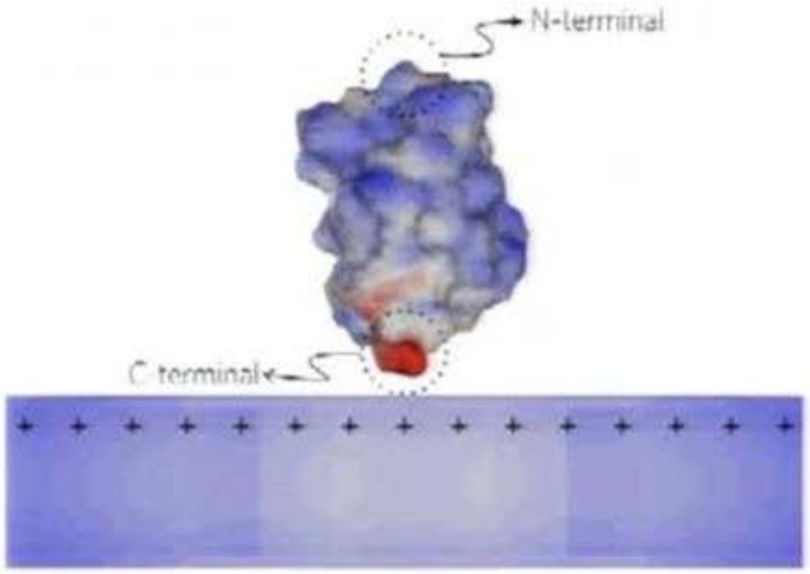
Antibody (or antibody-binding protein)

Preprint:

Probing protein orientation near charged surfaces with an implicit-solvent model and the PyGBe code

Christopher D. Cooper[1, a)] and Lorena A. Barba[2, b)]





Positive surface charge
NH_3^+ - SAM

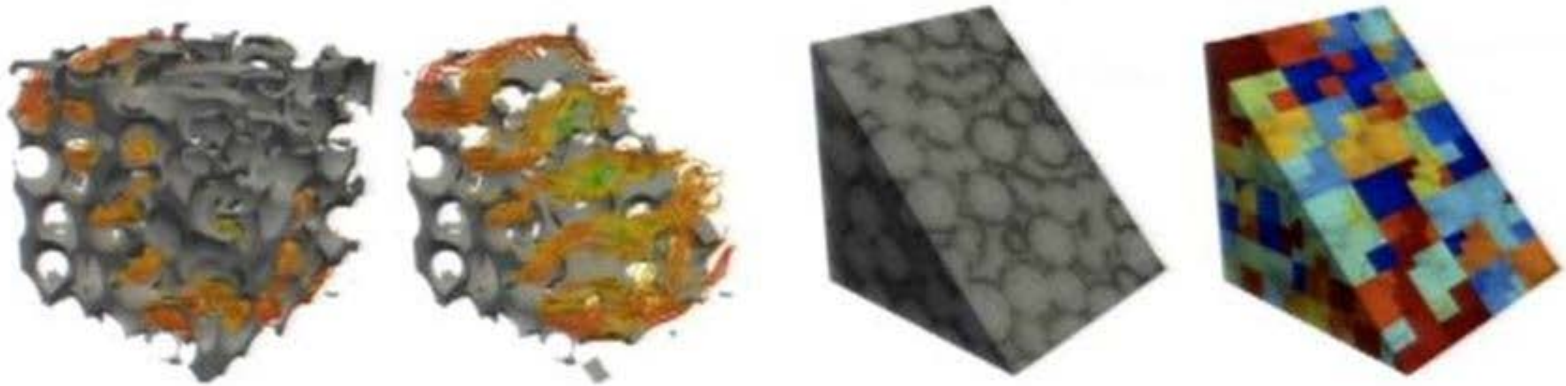
SC14: International Conference for High Performance Computing, Networking, Storage and Analysis

A volume integral equation Stokes solver for problems with variable coefficients

Dhairya Malhotra
The University of Texas at Austin,
Austin, TX 78712
dhairya.malhotra@gmail.com

Amir Gholami
The University of Texas at Austin,
Austin, TX 78712
i.amirgh@gmail.com

George Biros
The University of Texas at Austin,
Austin, TX 78712
gbiros@acm.org

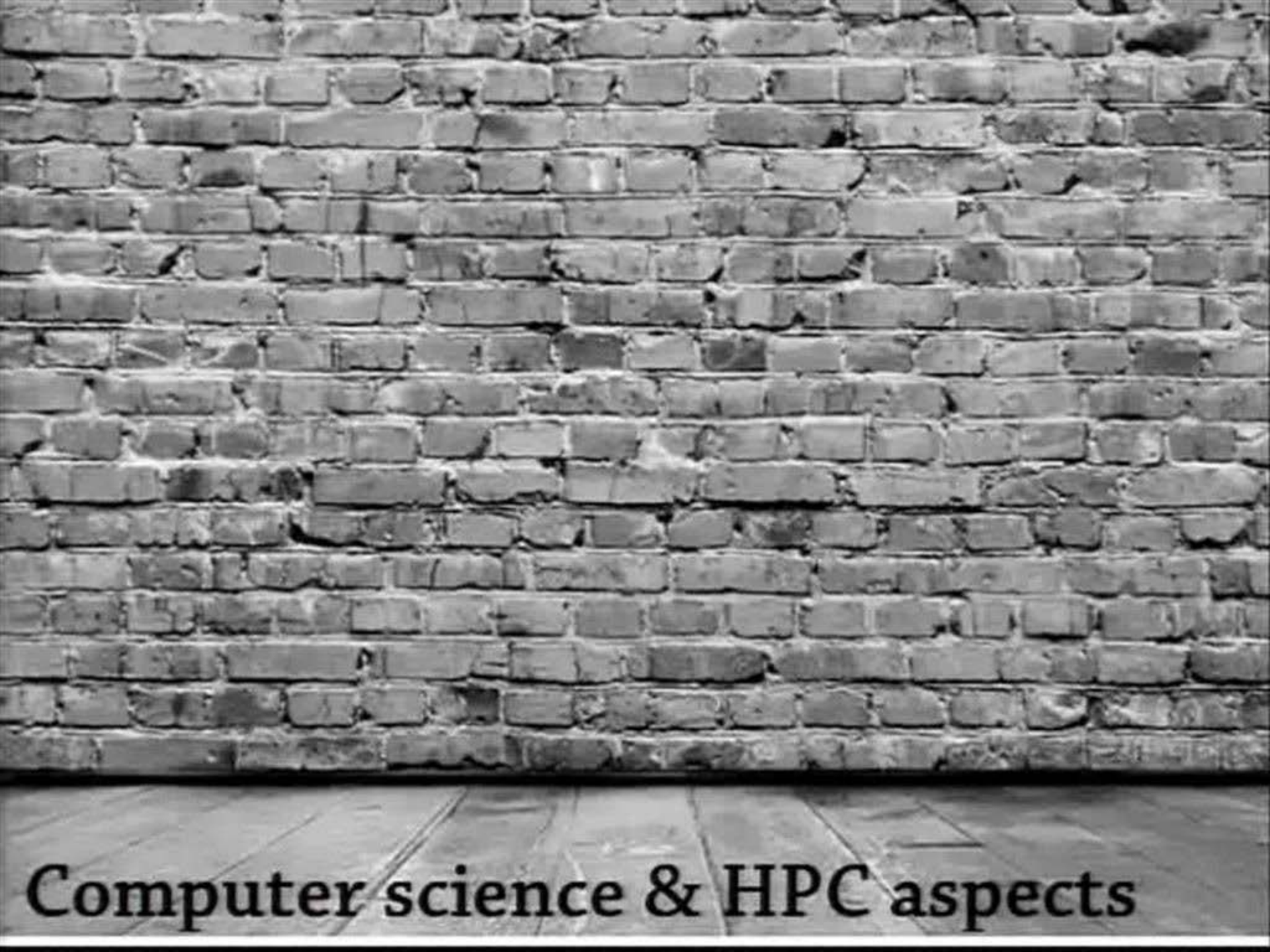


FAR-FIELD COMPRESSION FOR FAST KERNEL SUMMATION METHODS IN HIGH DIMENSIONS

WILLIAM B. MARCH* AND GEORGE BIROS

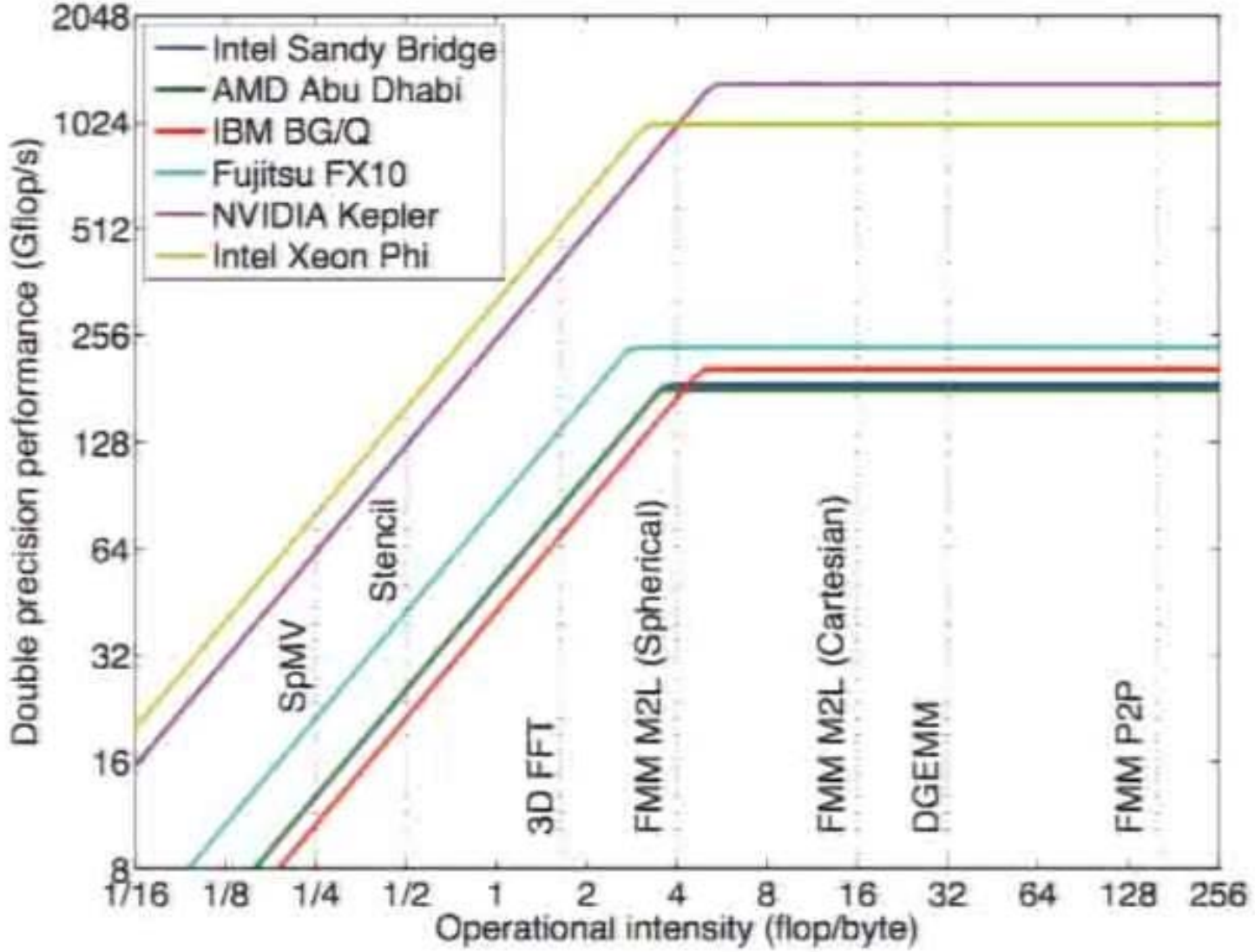
ASKIT: APPROXIMATE SKELETONIZATION KERNEL-INDEPENDENT TREECODE IN HIGH DIMENSIONS

WILLIAM B. MARCH*, BO XIAO*, AND GEORGE BIROS*


Computer science & HPC aspects

“Intensity trumps sparsity.”

see SIAM News, Vol. 46, No. 6, July/August 2013



Parallel FMM

- 1990 G&G — shared memory
- "A parallel adaptive fast multipole method", J. P. Singh, C. Holt, J. L. Hennessy, A. Gupta, Supercomputing '93 Proceedings of the 1993 ACM/IEEE Conference
- "Load Balancing and Data Locality in Adaptive Hierarchical N-Body Methods ...", J.P. Singh, C. Holt, T. Totsuka, A. Gupta, J. Hennessy, *Journal of Parallel and Distributed Computing*, 27(2):118-141 (1995)
- "A new parallel kernel-independent fast multipole method", L. Ying, G.Biros, D. Zorin, H. Langston, Supercomputing, 2003 ACM/IEEE Conference (***Best Student Paper Award***)

... jump to 2014

- Hybrid architectures & computational models

A CPU–GPU Hybrid Implementation and Model-Driven Scheduling of the Fast Multipole Method

Jee Choi[1], Aparna Chandramowlishwaran[3], Kamesh Madduri[4], Richard Vuduc[2]

A Performance Model for the Communication in Fast Multipole Methods on HPC Platforms

Huda Ibeid, Rio Yokota, and David Keyes

Communication Complexity of the Fast Multipole Method and its Algebraic Variants

Rio Yokota[1], *George Turkiyyah*[1], *David Keyes*[1]

Reference	Processes		Data per Process		Communication complexity
Teng [32]	$\mathcal{O}(P)$		$\mathcal{O}\left((N/P)^{2/3}(\log N+\mu)^{1/3}\right)$		$\mathcal{O}\left(P(N/P)^{2/3}(\log N+\mu)^{1/3}\right)$
Lashuk *et al.* [27]	$\mathcal{O}(\sqrt{P})$		$\mathcal{O}\left((N/P)^{2/3}\right)$		$\mathcal{O}\left(\sqrt{P}(N/P)^{2/3}\right)$
Ibeid *et al.* [21]	Global	Local	Global	Local	Global + Local
	$\mathcal{O}(\log P)$	$\mathcal{O}(1)$	$\mathcal{O}(1)$	$\mathcal{O}\left((N/P)^{2/3}\right)$	$\mathcal{O}\left(\log P+(N/P)^{2/3}\right)$

From *SIAM News*, Volume 46, Number 6, July/August 2013

CSE 2013

How Will the Fast Multipole Method Fare in the Exascale Era?

By Lorena A. Barba and Rio Yokota

Another cause for optimism is the new spirit of collaboration emerging in the field. Leading up to the SIAM CSE conference, several groups were exchanging ideas about building a set of standard benchmark tests for FMM codes and, in due course, developing a community software library. A handful of open-source codes are already available, but adoption of multipole algorithms would thrive if we had a BLAS-like col-

Open-source codes

- 2004, updated 2006

KIFMM3d Download and Installation

Home Download and Installation Documentation Publications Links Contact

The Kernel-Independent Fast Multipole (FMM) 3D code (kifmm3d) requires the installation of several libraries. Before downloading the kifmm3d code, make sure to install the necessary libraries listed on the links page.

Download

The most current version of the code and documentation can be downloaded here

- Code: kifmm3d.tar.gz
- HTML Documentation: kifmm3d_doc.tar.gz(Not yet active)

Open-source codes

- 2010

INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING
Int. J. Numer. Meth. Engng 2011; **85**:403–428
Published online 1 September 2010 in Wiley Online Library (wileyonlinelibrary.com). DOI: 10.1002/nme.2972

PetFMM—A dynamically load-balancing parallel fast multipole library

Felipe A. Cruz[1], Matthew G. Knepley[2] and L. A. Barba[3,*,†]

Open-source codes

- 2012: ExaFMM.org

Boston University Mechanical Engineering
ExaFMM

DOWNLOAD FUNDING REFERENCES DOCUMENTATION NEWS CONTACT US

License

For maximum freedom of use, **ExaFMM is distributed under** The MIT License (MIT). Please note that you must give proper attribution in all derived works.

> *Copyright © 2011 L Barba & R Yokota*
>
> *Permission is hereby granted, free of charge, to any person obtaining a copy of this software and associated documentation files (the "Software"), to deal in the Software without restriction, including without limitation the rights to use, copy, modify, merge, publish, distribute, sublicense, and/or sell copies of the Software, and to permit persons to whom the Software is furnished to do so, subject to the following conditions:*
>
> *The above copyright notice and this permission notice shall be included in all copies or substantial portions of the Software.*

Download

License

Related Links

Barba group

Vuduc HPC Garage

Open-source codes

- 2013

A CPU–GPU Hybrid Implementation and Model-Driven Scheduling of the Fast Multipole Method

Jee Choi[1], Aparna Chandramowlishwaran[3], Kamesh Madduri[4], Richard Vuduc[2]

Open-source codes

- 2014: PvFMM.org

A volume integral equation Stokes solver for problems with variable coefficients

Dhairya Malhotra
The University of Texas at Austin,

Amir Gholami
The University of Texas at Austin,

George Biros
The University of Texas at Austin,

Can we coalesce an open community?