Using GPUs for the Boundary Element Method

Christopher Cooper
Lorena Barba
Boston University

November, 2011

Pan-American Advanced Studies Institute
NSF Program

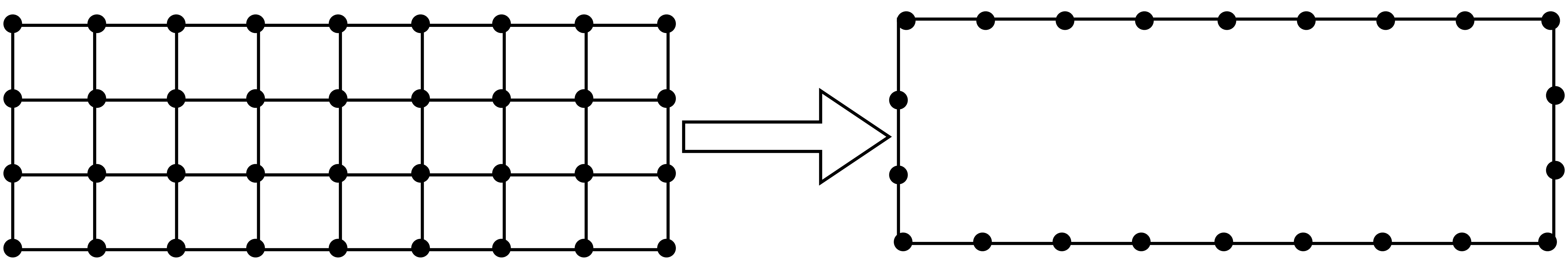
BU College of Engineering

Boundary Element Method - Formulation

- Numerical Method for PDEs

$$\nabla^2\phi(\mathbf{x}) \quad \Longrightarrow \quad \phi(\mathbf{x}) = \int_\Gamma \psi(\mathbf{x},\mathbf{x}')\,d\Gamma'$$

Only on boundary!

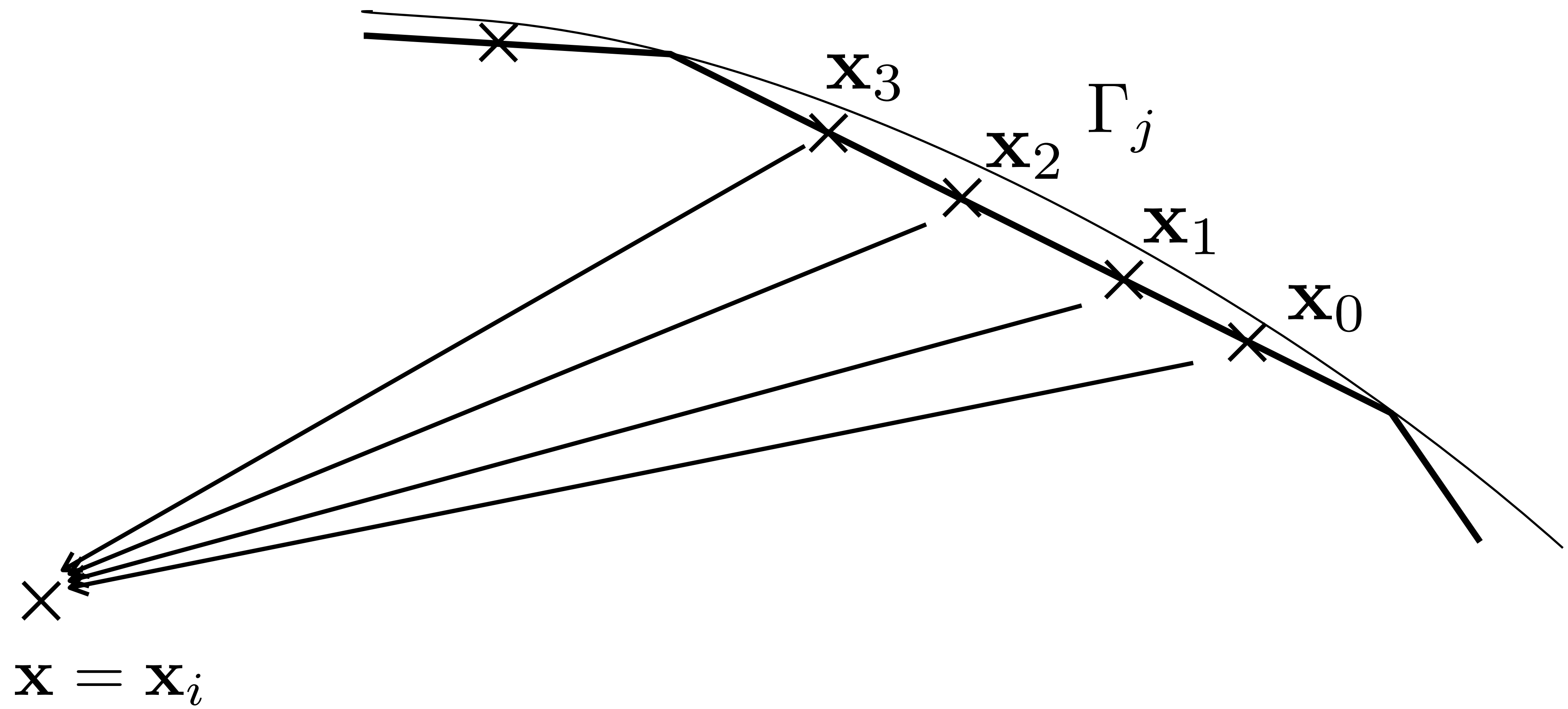


Volume mesh

Surface mesh

Boundary Element Method - Matrix Formulation

- Apply for all boundary elements at $\mathbf{x} = \mathbf{x}_i$



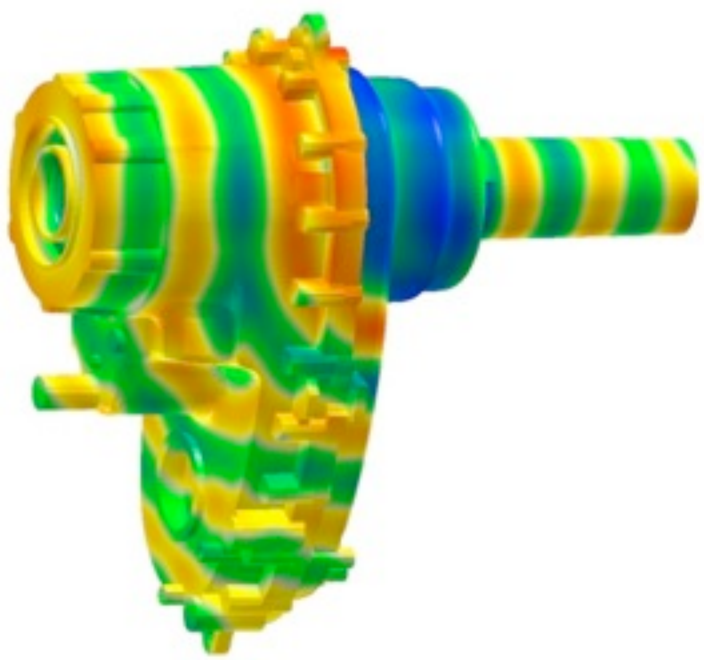
$$[A]\{X\} = [B]\{Y\}$$

$\{X\}$ unknown boundary values

$\{Y\}$ known boundary values

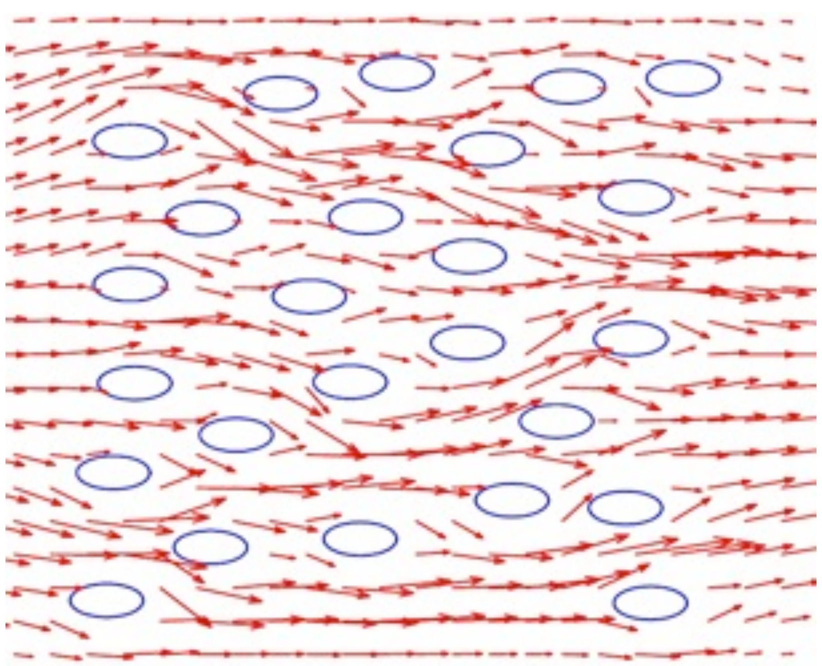
Boundary Element Method - Applications

Acoustics



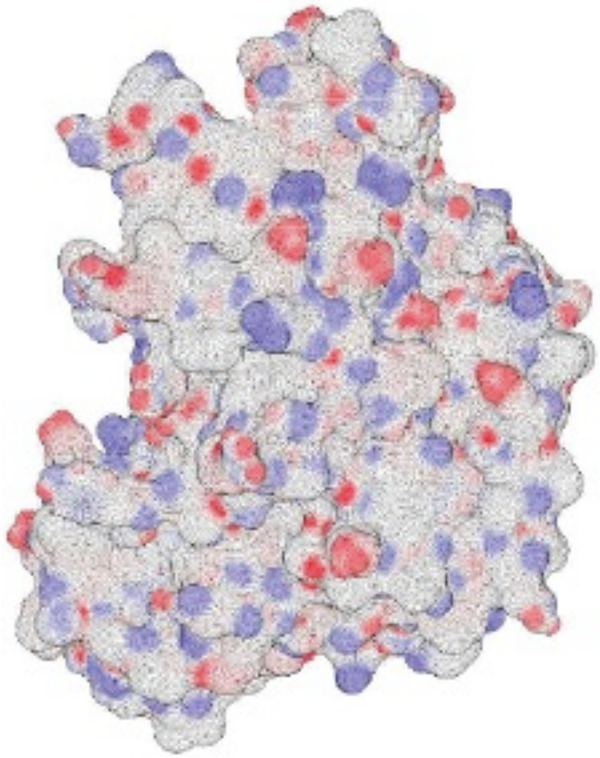
Advanced Numerical Solutions
ansol.us

Stokes flow



FastBEM
urbana.mie.uc.edu

Electrostatics



Yokota et al. 2011

Boundary Element Method - Limitations

- Dense matrix vector multiplications scale as $O(N^2)$!
  - Assembling the RHS

$$[B]\,\{Y\} = \{b\}$$

  - Krylov subspace linear solver (GMRES, CG, …)

$$[A]\,\{X\} = \{b\}$$

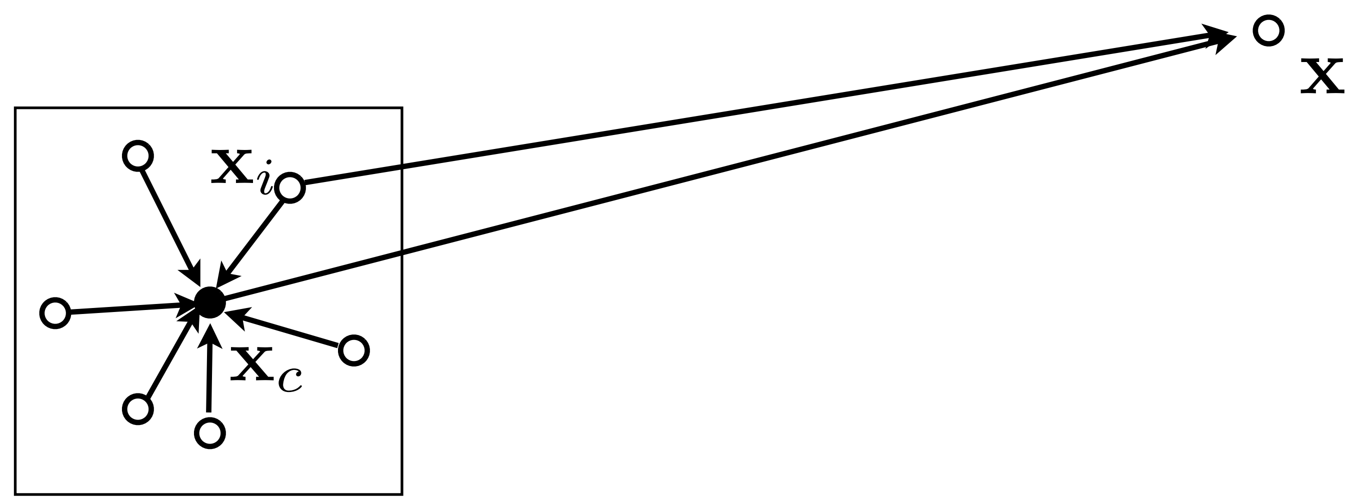
Naive approach allows for only a few thousand elements!

Fast Multipole Method (FMM)

- Fast interaction calculation algorithm

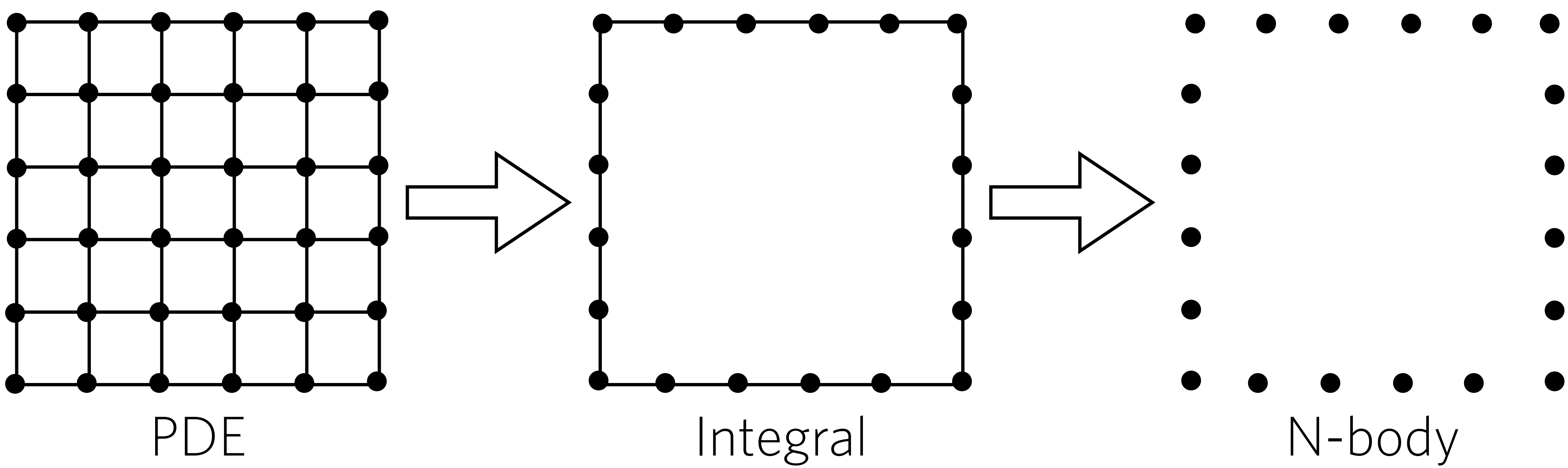
$$\phi(\mathbf{x}) = \sum_{i=0}^{N-1} \alpha_i \psi(|\mathbf{x} - \mathbf{x}_i|)$$

- Approximates far field



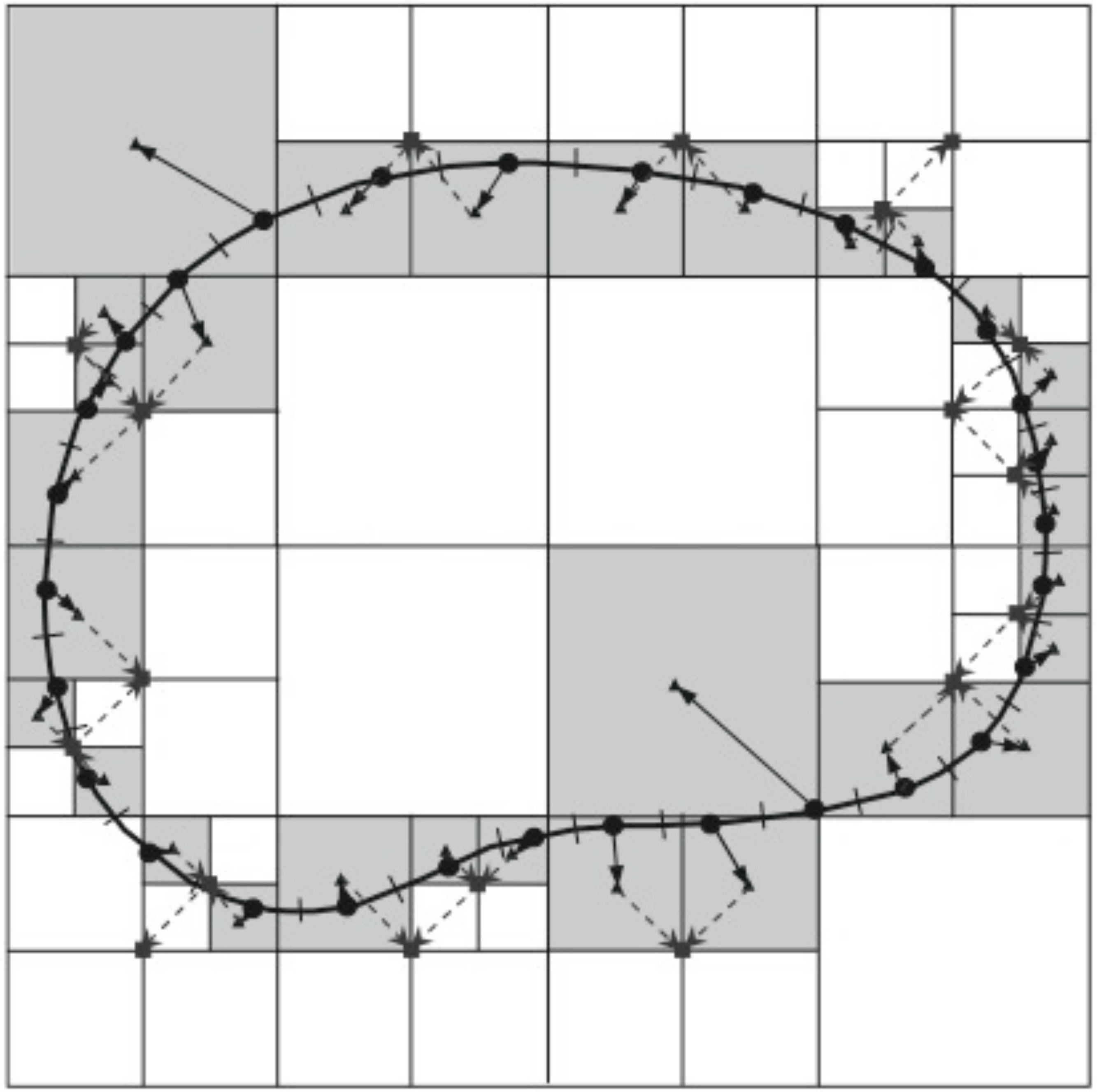
BEM - FMM

- BEM Matrix vector multiplications are interaction calculations



$$\phi(\mathbf{x}) = \sum_{i=0}^{N-1} \alpha_i G(|\mathbf{x} - \mathbf{x}_i|)$$

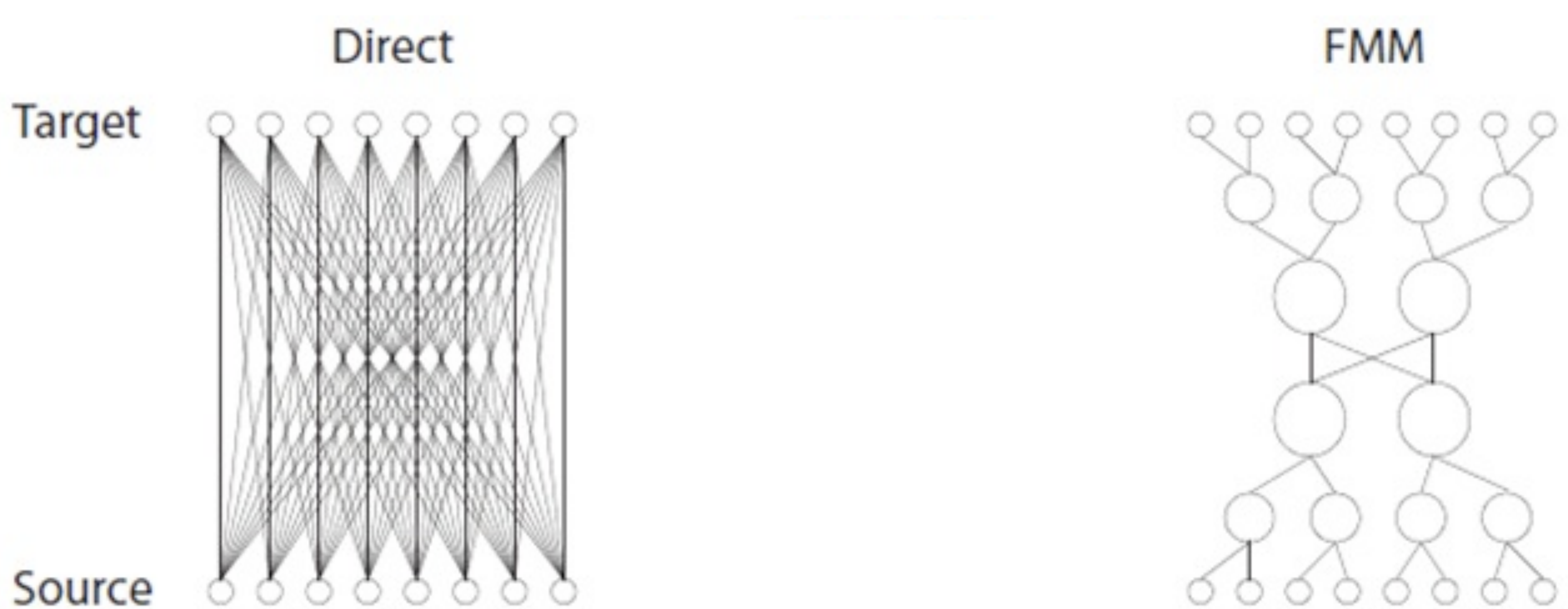
BEM - FMM



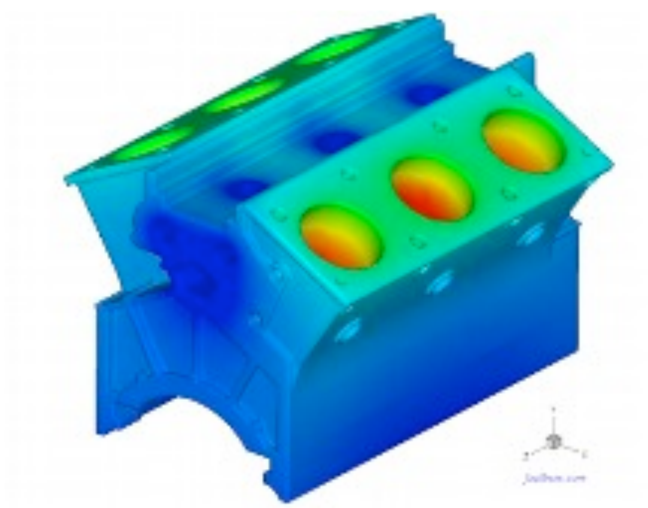
Liu . Fast Multipole Boundary Element Method

BEM - FMM

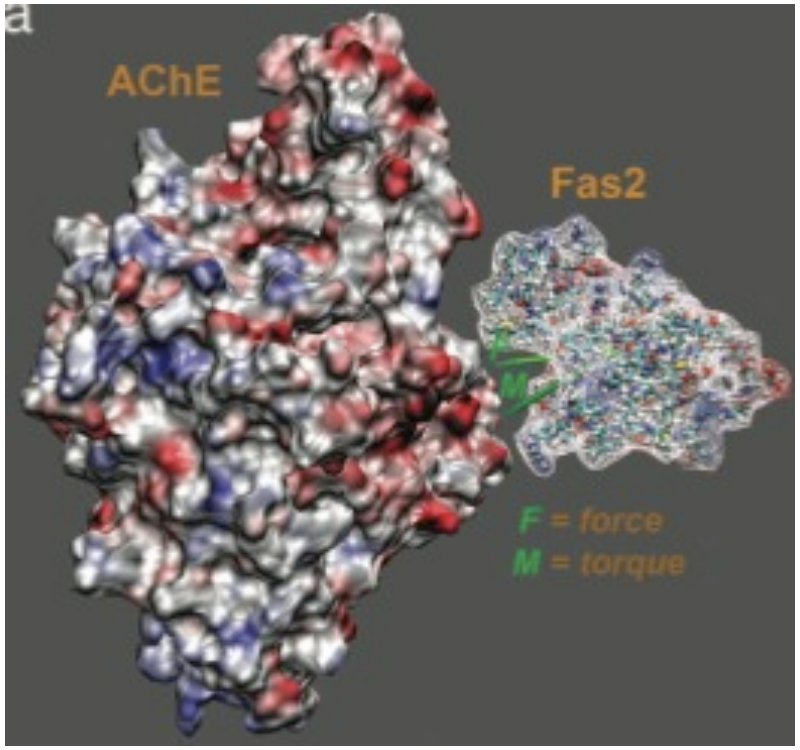
- Accelerates matrix vector computation:
  - Far field is approximated -> O(N) calculations
- No need to store the matrix
  - Values computed on the fly -> O(N) storage



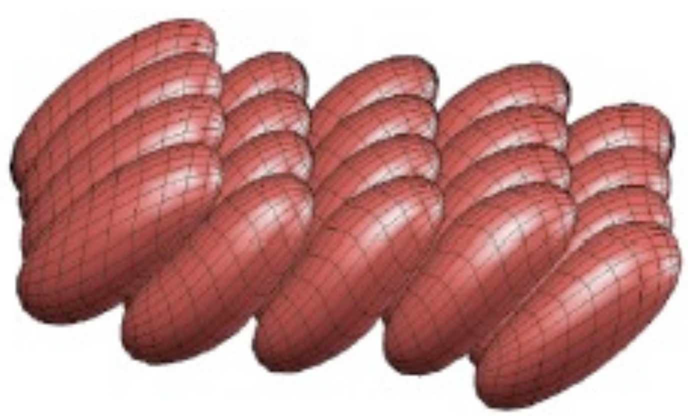
BEM FMM - Previous work



Fast BEM



Lu et al.



“Petascale direct numerical simulation of blood flow on 200K cores and heterogeneous architectures”

Rahimian et al.

BEM FMM and GPUs

- BEM and FMM provide an important reduction in computation

BEM

Mesh reduction

FMM

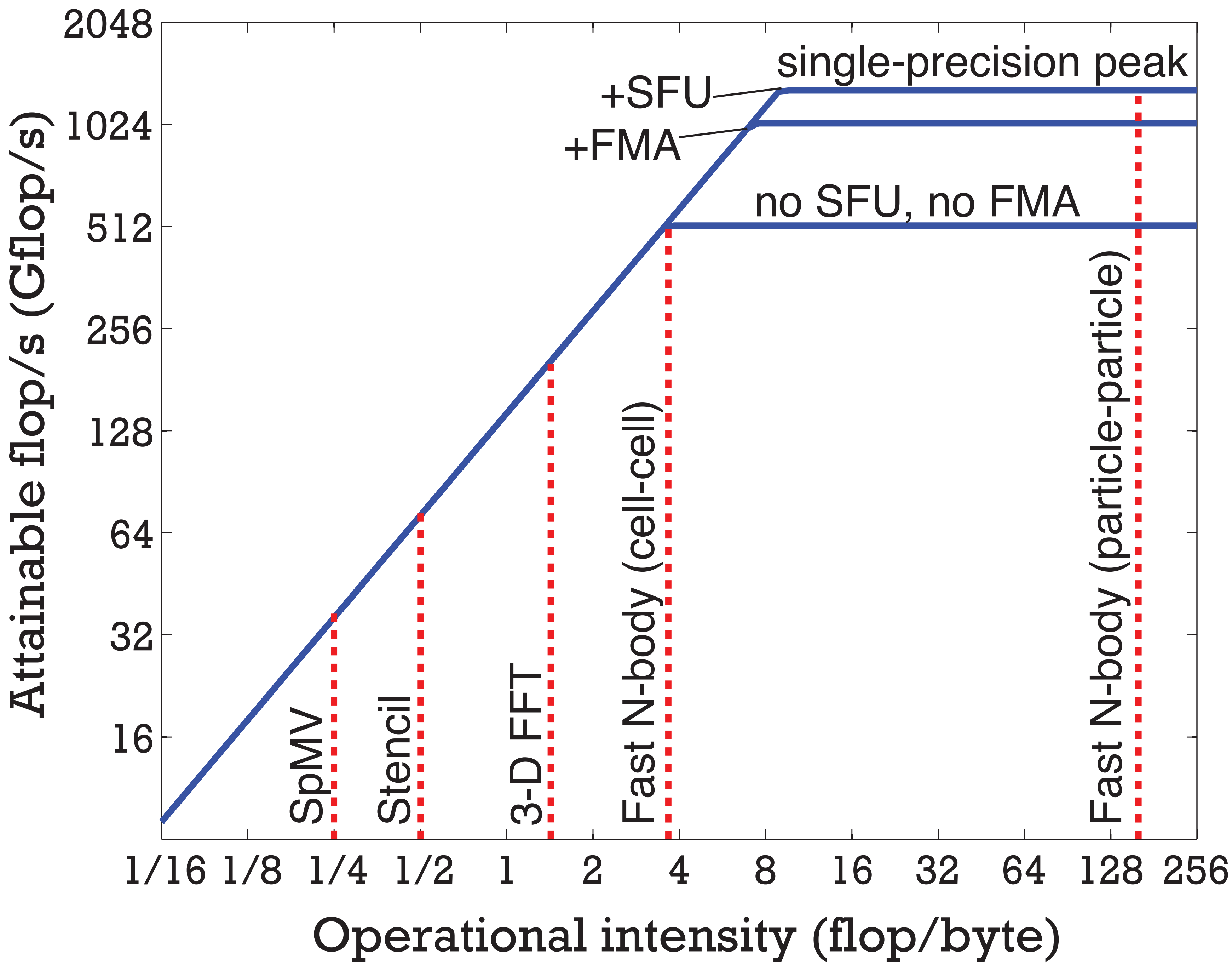
Reduce computation

Look for further reduction from hardware!

GPU

BEM FMM and GPUs

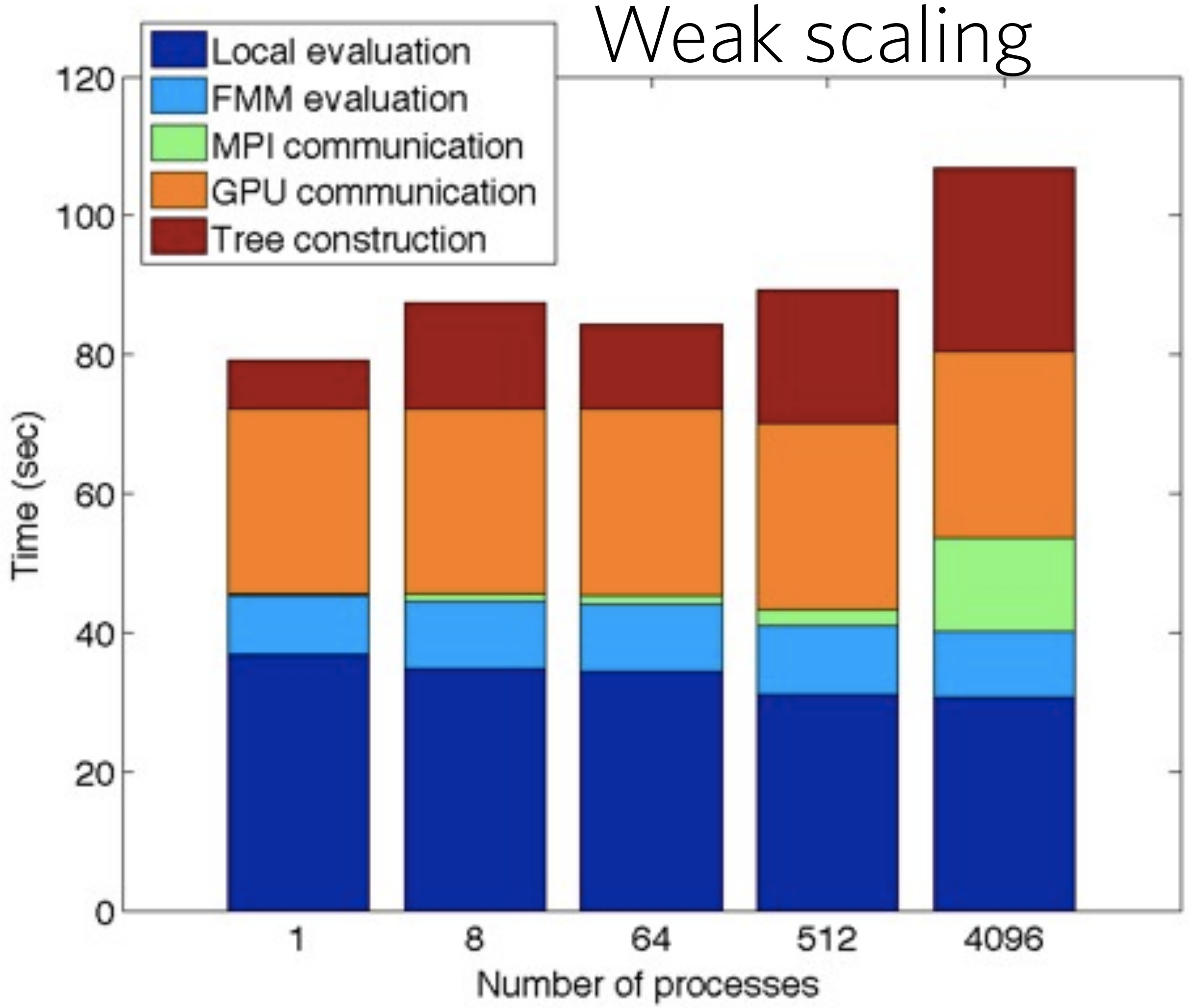
- FMM maps well to GPUs



FMM - Available resources

- ExaFMM: FMM library that runs on GPUs
  - Shown to scale well to thousands of GPUs
  - Performs in the order of Peta FLOPS

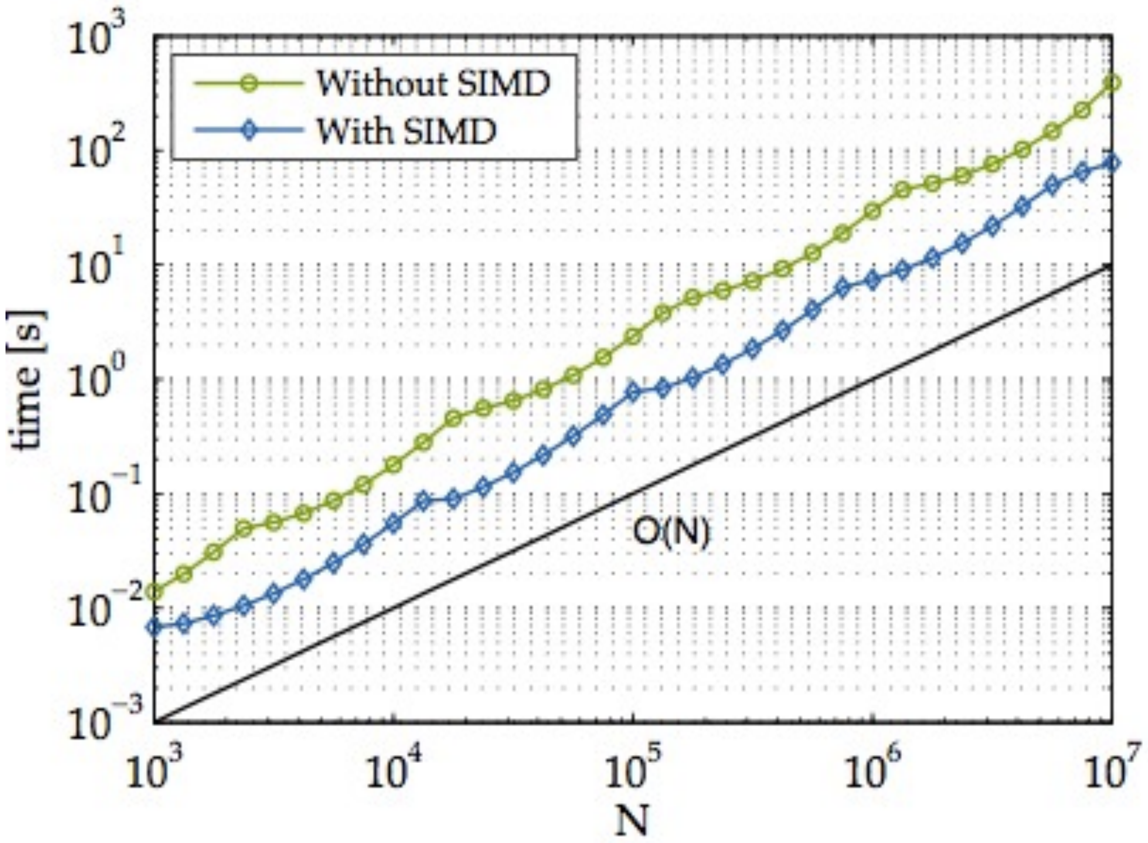
Weak scaling

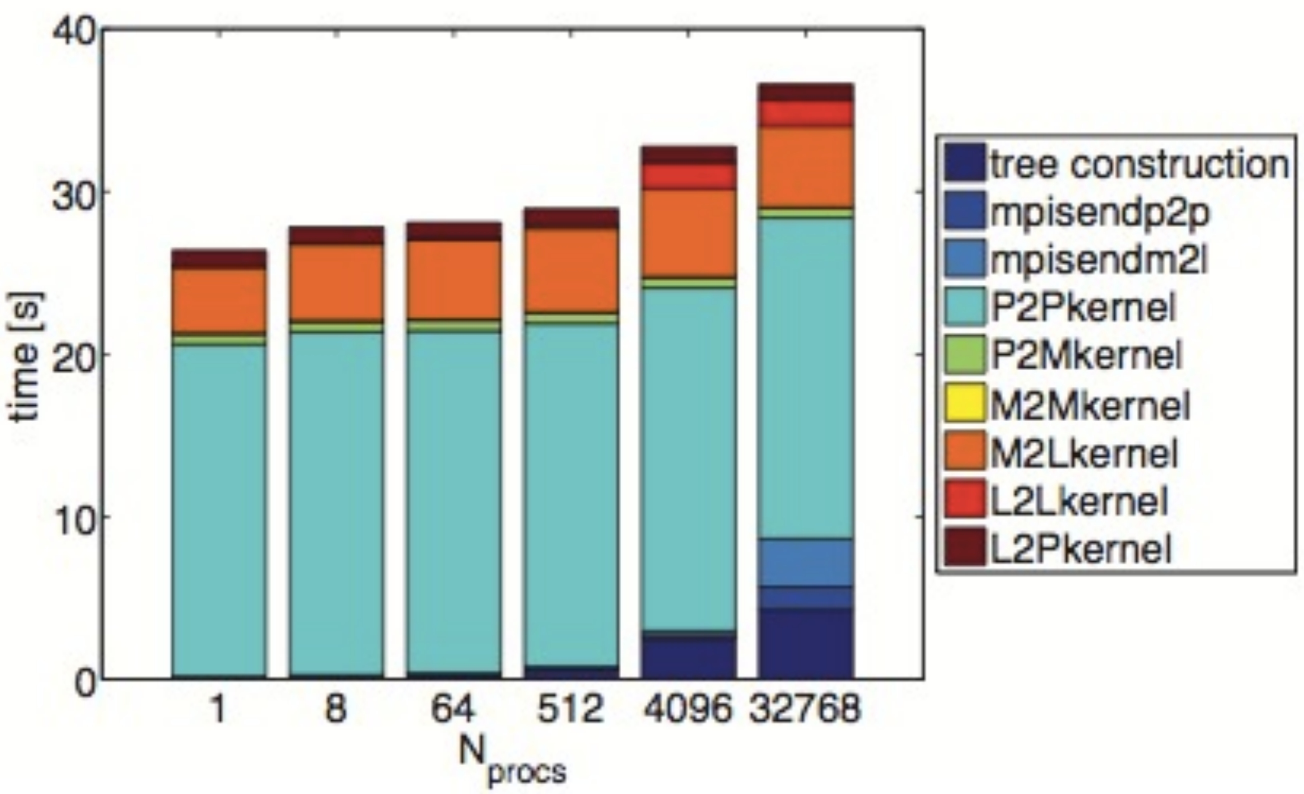


64 billion in 100 seconds
1.0 PFlops
4K GPUs on TSUBAME

FMM - Available resources

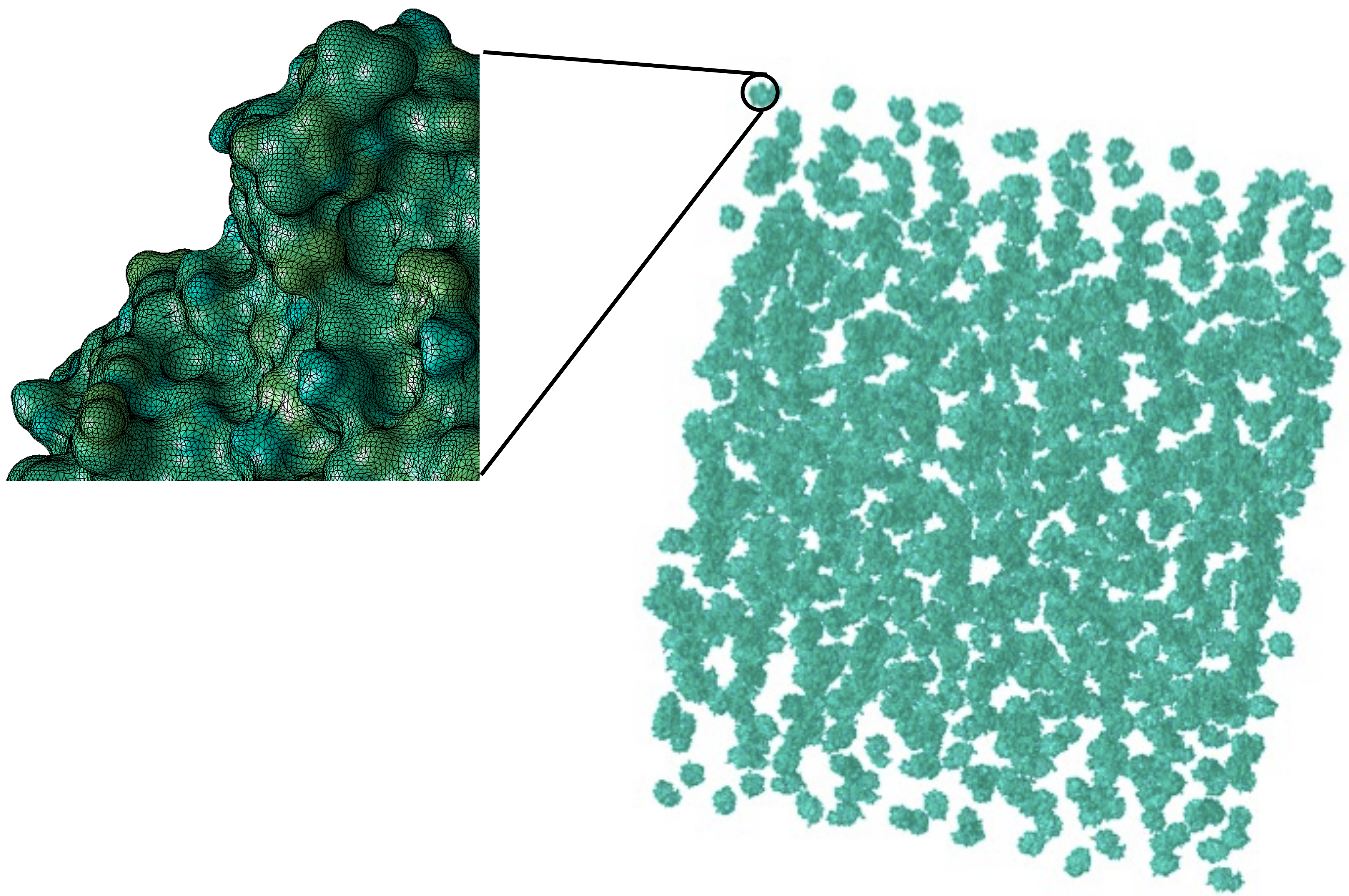
- ExaFMM: an **open source** FMM library that runs on GPUs
  - Released in SC'11





How far can we go?

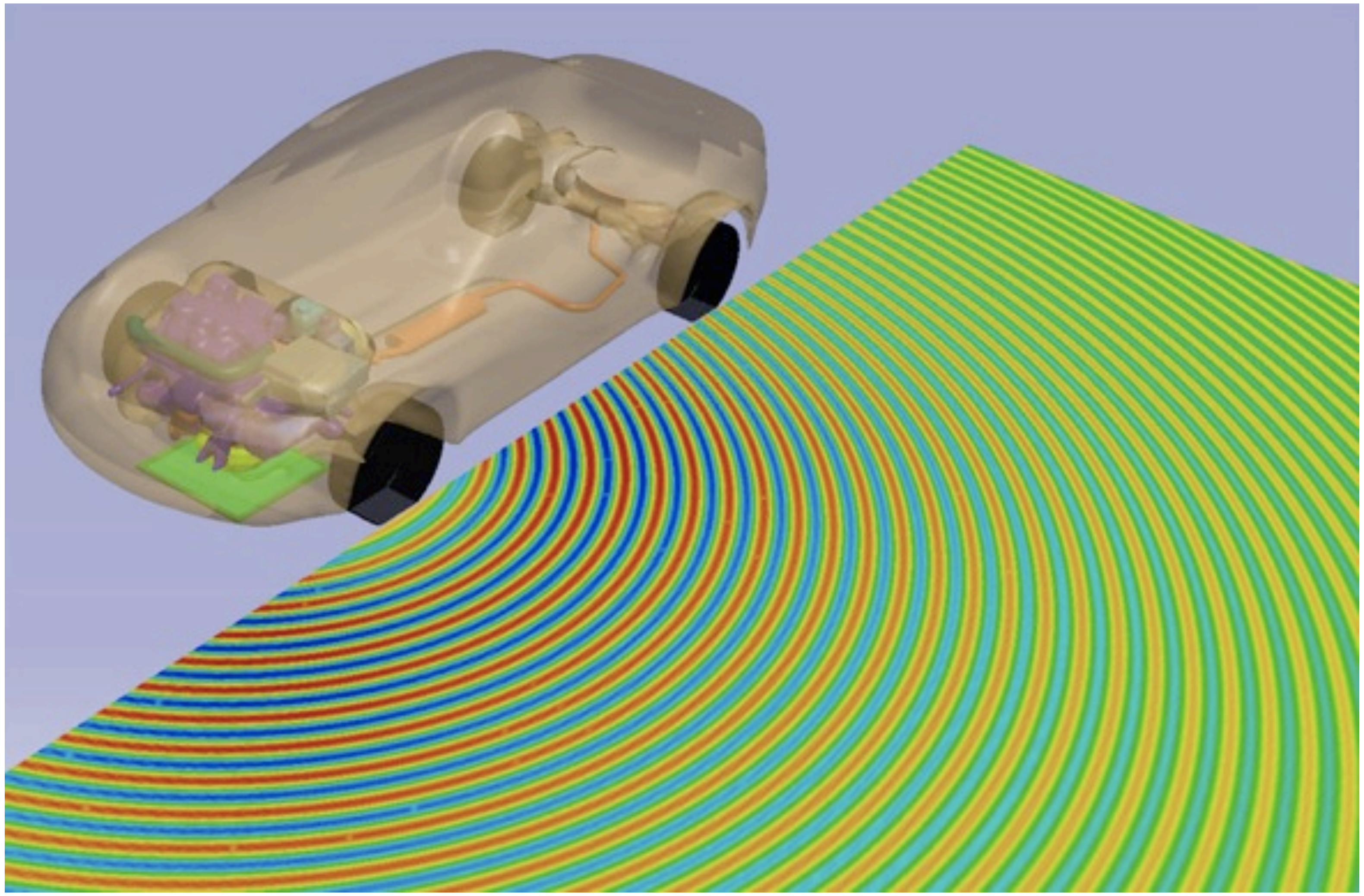
- Bioelectrostatics



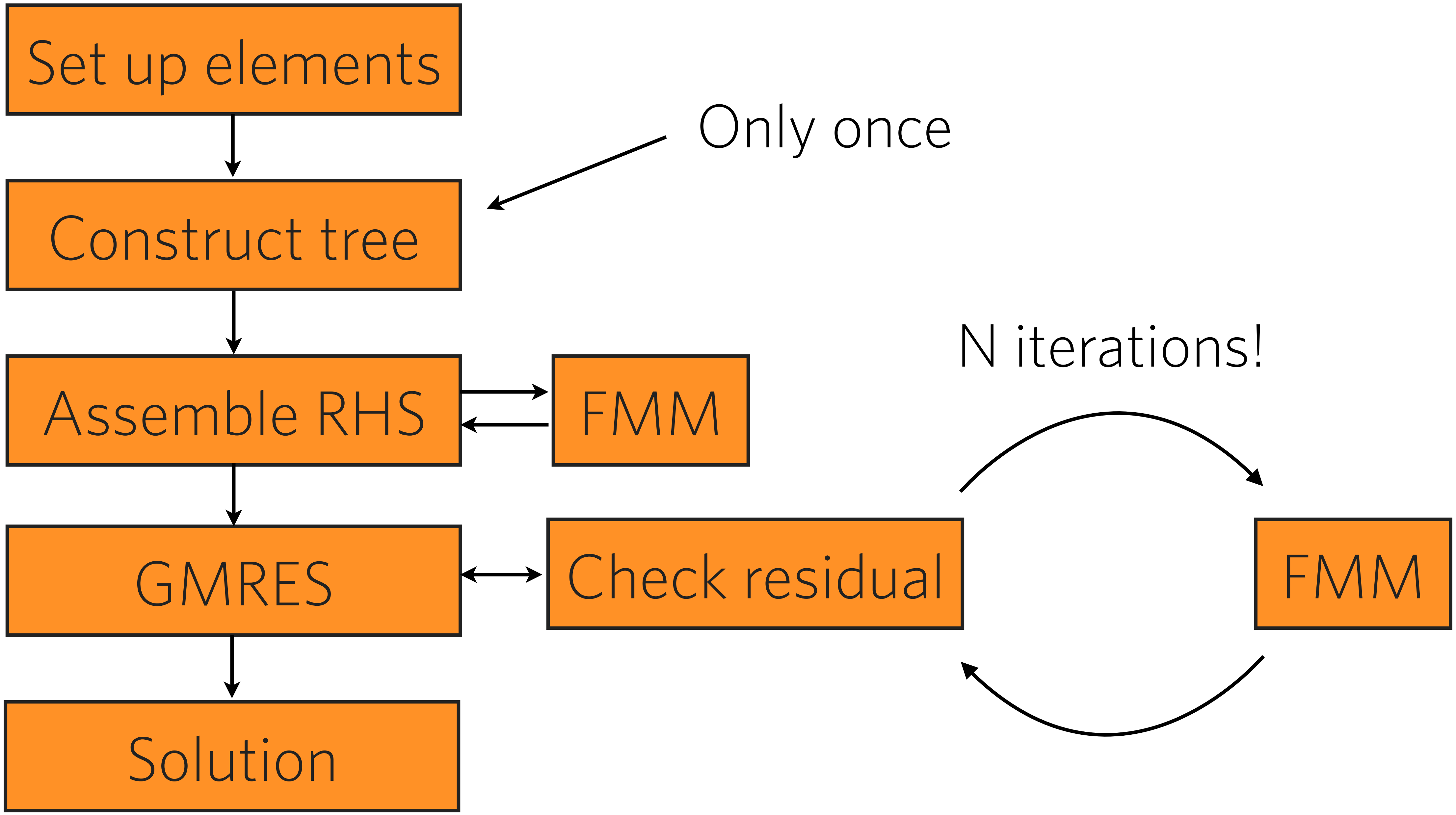
Billions of elements!

How far can we go?

- Acoustics
  - Helmholtz equation solved for each frequency

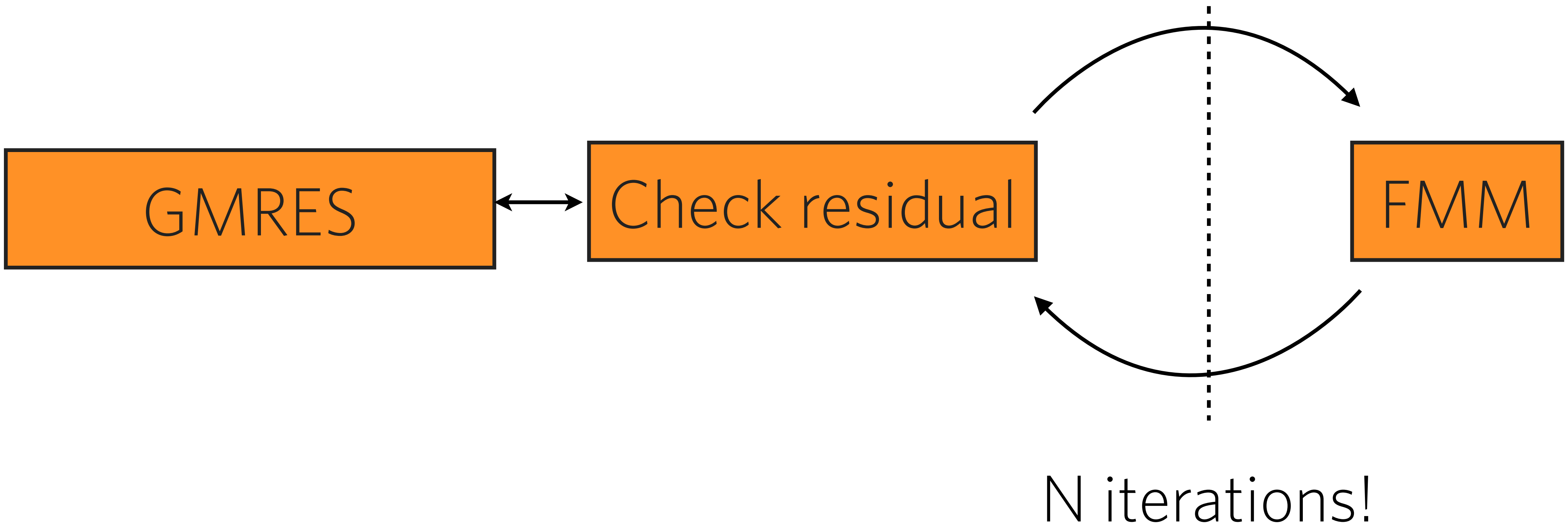


FMM BEM - Implementation



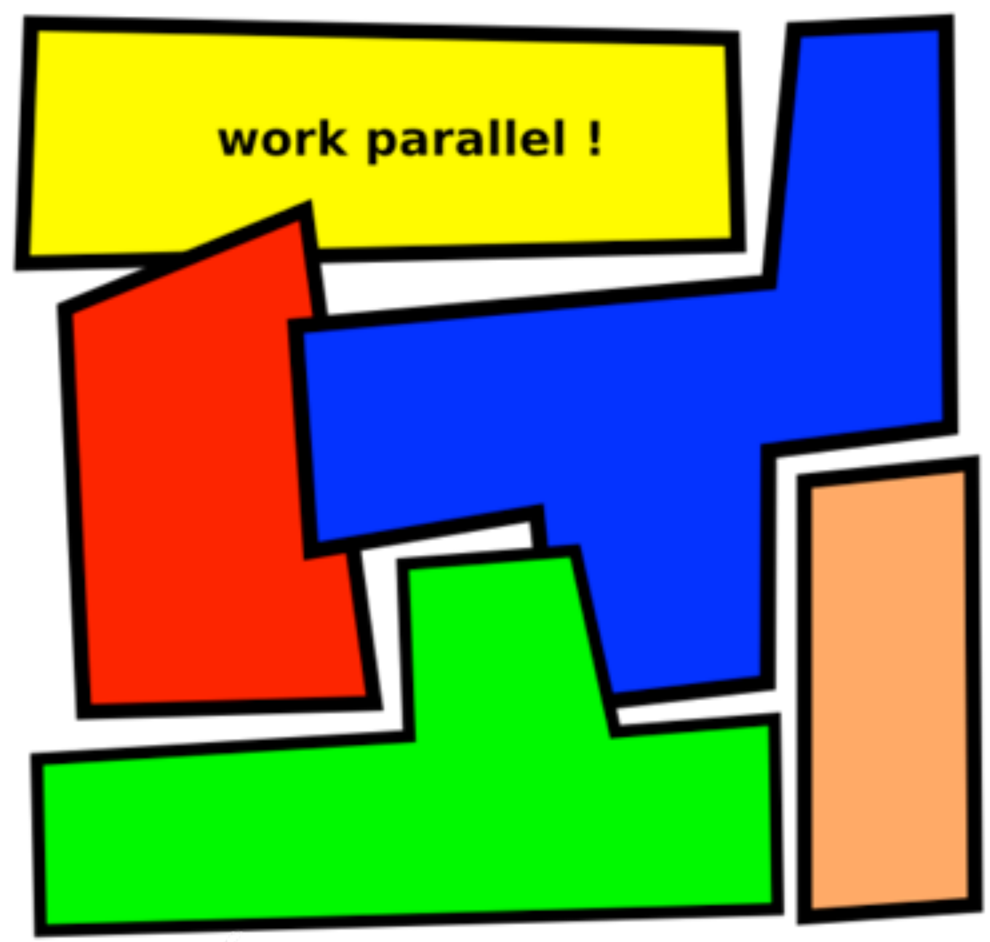
Main challenges

- Porting the whole BEM to the GPU
  - Avoid excessive CPU-GPU communication



Main challenges

- Constructing a BEM in the ExaFMM framework
  - Needed for large number of elements
  - Use ExaFMM's domain decomposition for parallelization



Conclusions and future work

- BEM FMM technology is a very good candidate to be accelerated with GPUs

- Intelligent use of tools such as ExaFMM will allow us to solve cool engineering problems!