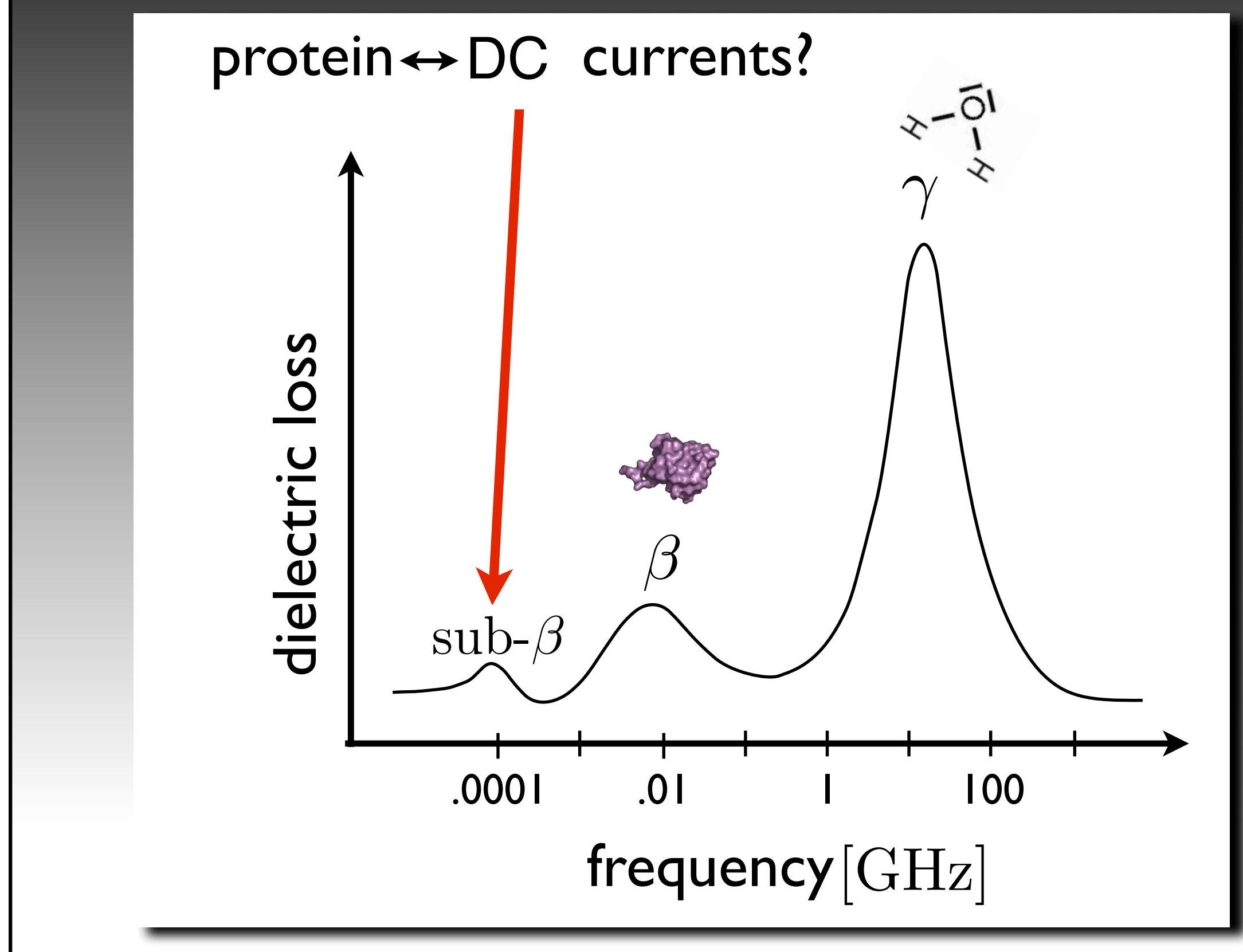
CUDA Acceleration of MG-FEM-BEM Methods for Dielectric Interfaces

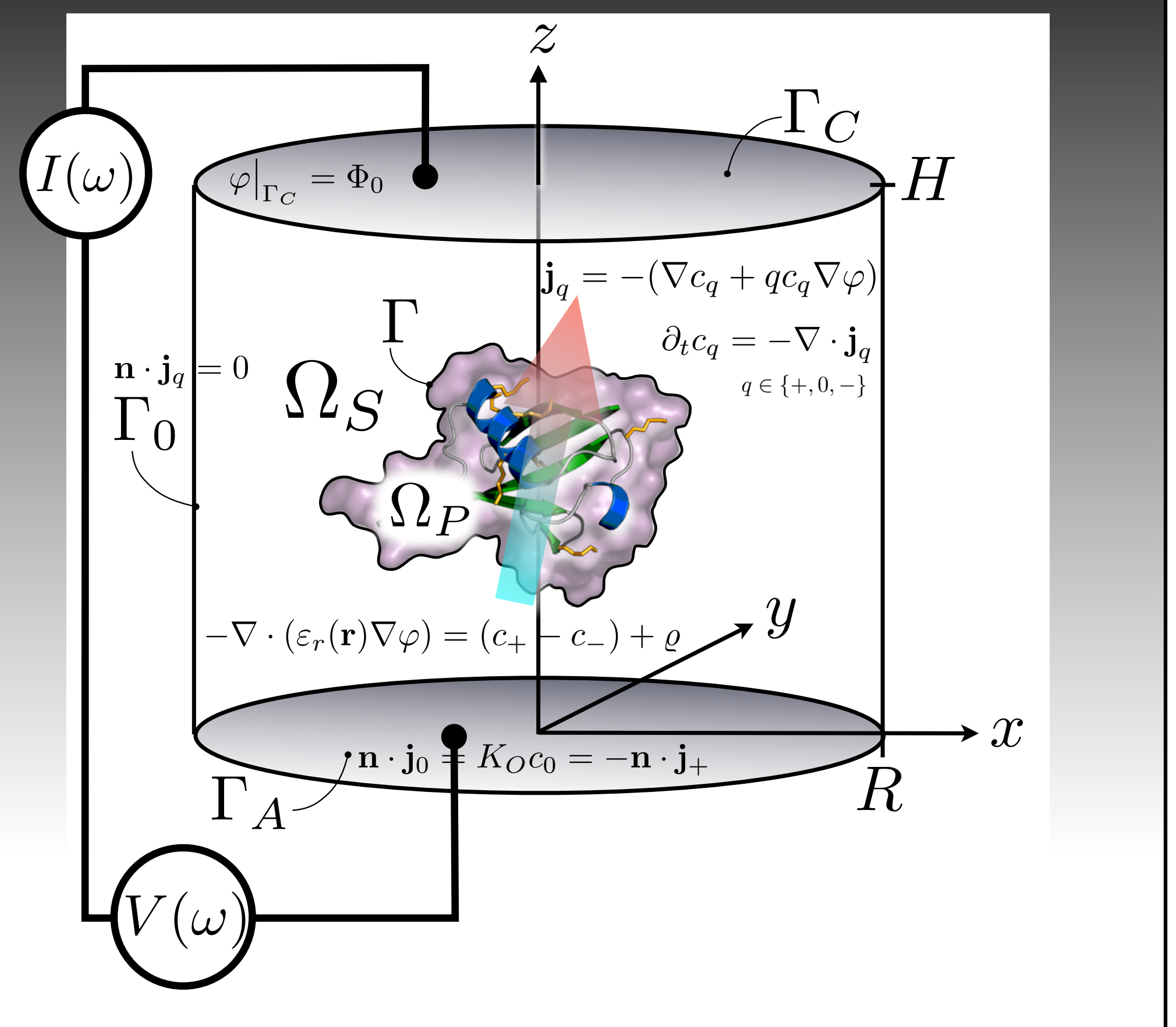
Christian Holme

Betreuer: Stephan Kramer, Johannes Hagemann, Gert Lube

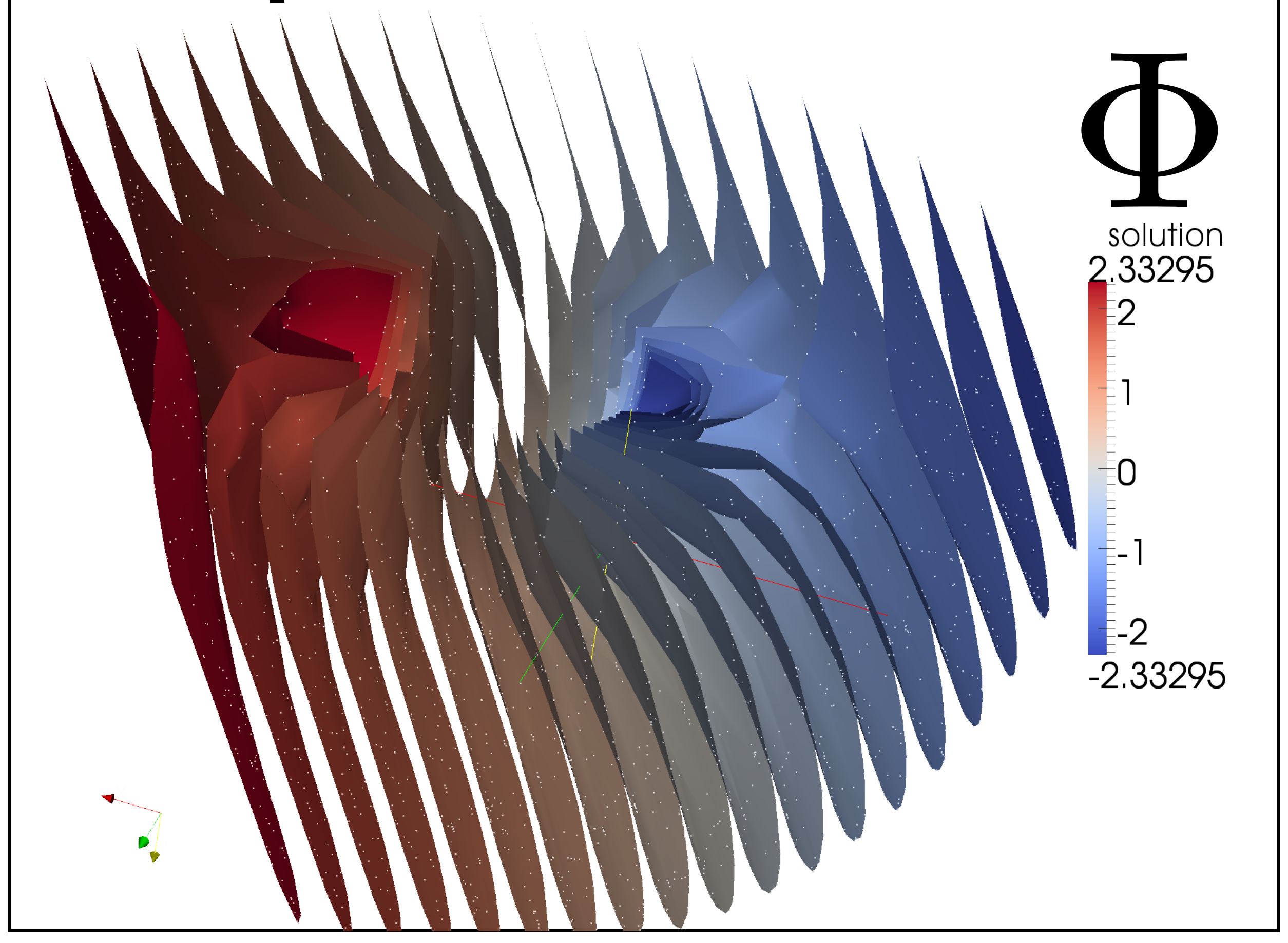
Institut f. Numerische und Angewandte Mathematik | CUDA Lab Course 2013 | Georg-August-Universität Göttingen

Dielectric Relaxation of Proteins




z
y
x
H
R
Γ_C
Γ_0
Γ_A
Γ
Ω_S
Ω_P
$I(\omega)$
$V(\omega)$
$\varphi|_{\Gamma_C} = \Phi_0$
$\mathbf{j}_q = -(\nabla c_q + q c_q \nabla\varphi)$
$\partial_t c_q = -\nabla\cdot\mathbf{j}_q$
$q \in \{+,0,-\}$
$\mathbf{n}\cdot\mathbf{j}_q = 0$
$-\nabla\cdot(\varepsilon_r(\mathbf{r})\nabla\varphi) = (c_+ - c_-) + \varrho$
$\mathbf{n}\cdot\mathbf{j}_0 = K_O c_0 = -\mathbf{n}\cdot\mathbf{j}_+$

Dipole Isosurfaces



FEM-BEM Assembly Parallelization

(A) FEM : 12 QThreads + CUDA for BEM

(B) FEM : 1 QThread + CUDA for BEM

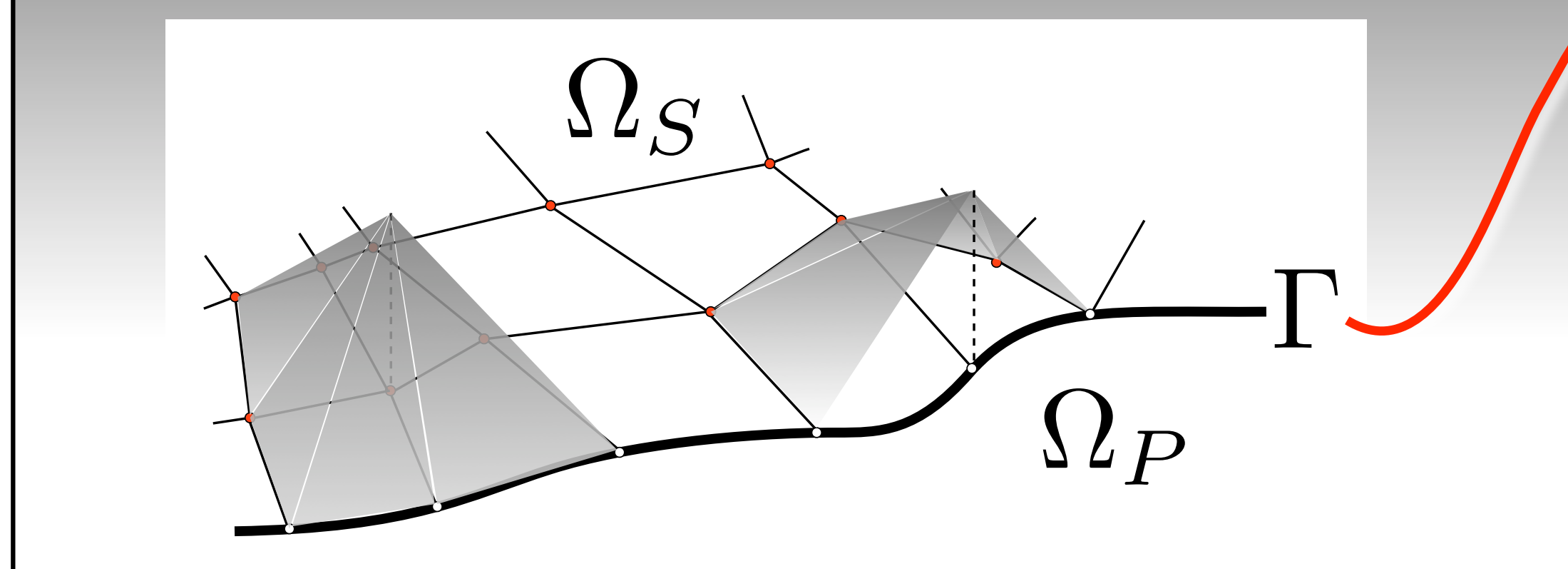
(C) FEM+BEM : 12 QThreads

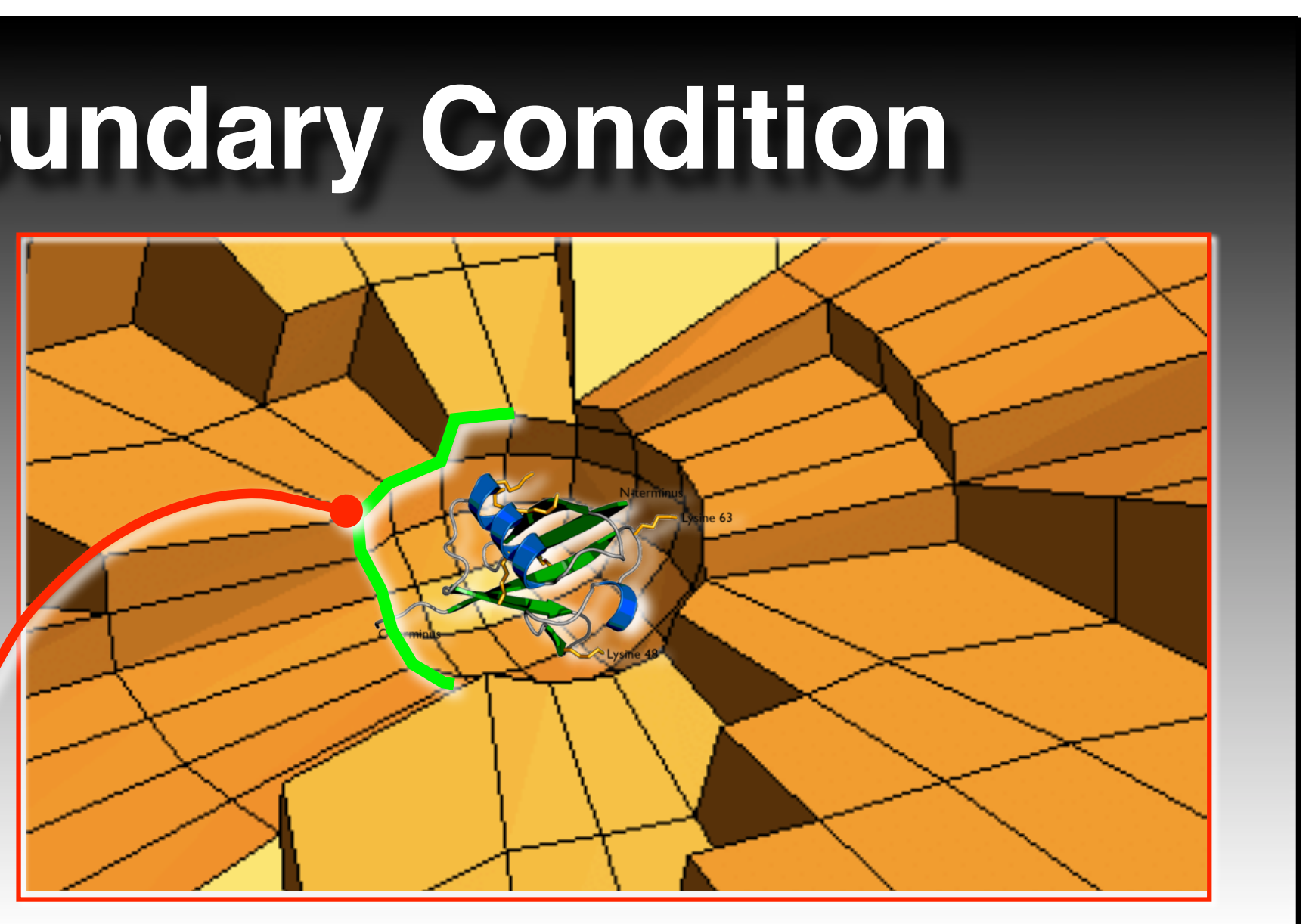
(D) FEM+BEM : 1 QThread

Protein as Non-local Boundary Condition

FEM

$$-\nabla\cdot(\varepsilon_S\nabla\Phi) = 0 \ + \ BC$$



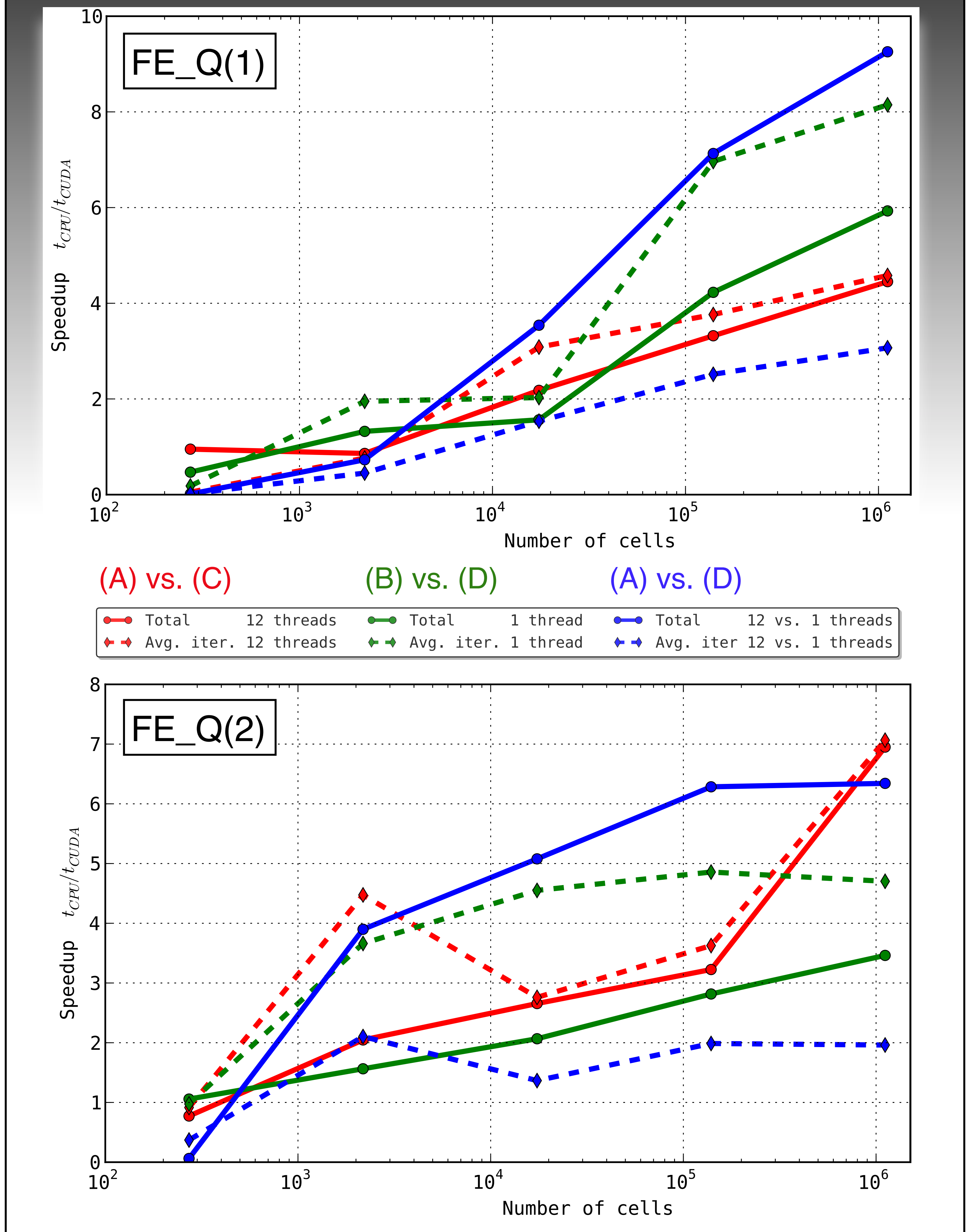


BEM

$$\frac{1}{2}\Phi(\mathbf{x}) + \oint_\Gamma \left[\Phi(\mathbf{x}')\frac{\partial G_\mathbf{x}}{\partial \mathbf{n}'}(\mathbf{x}') - G_\mathbf{x}(\mathbf{x}')\frac{\varepsilon_S}{\varepsilon_P}\frac{\partial\Phi}{\partial\mathbf{n}'}\right] = \phi^C(\mathbf{x})$$

Speedup

4th order surface & BEM quad. order 8

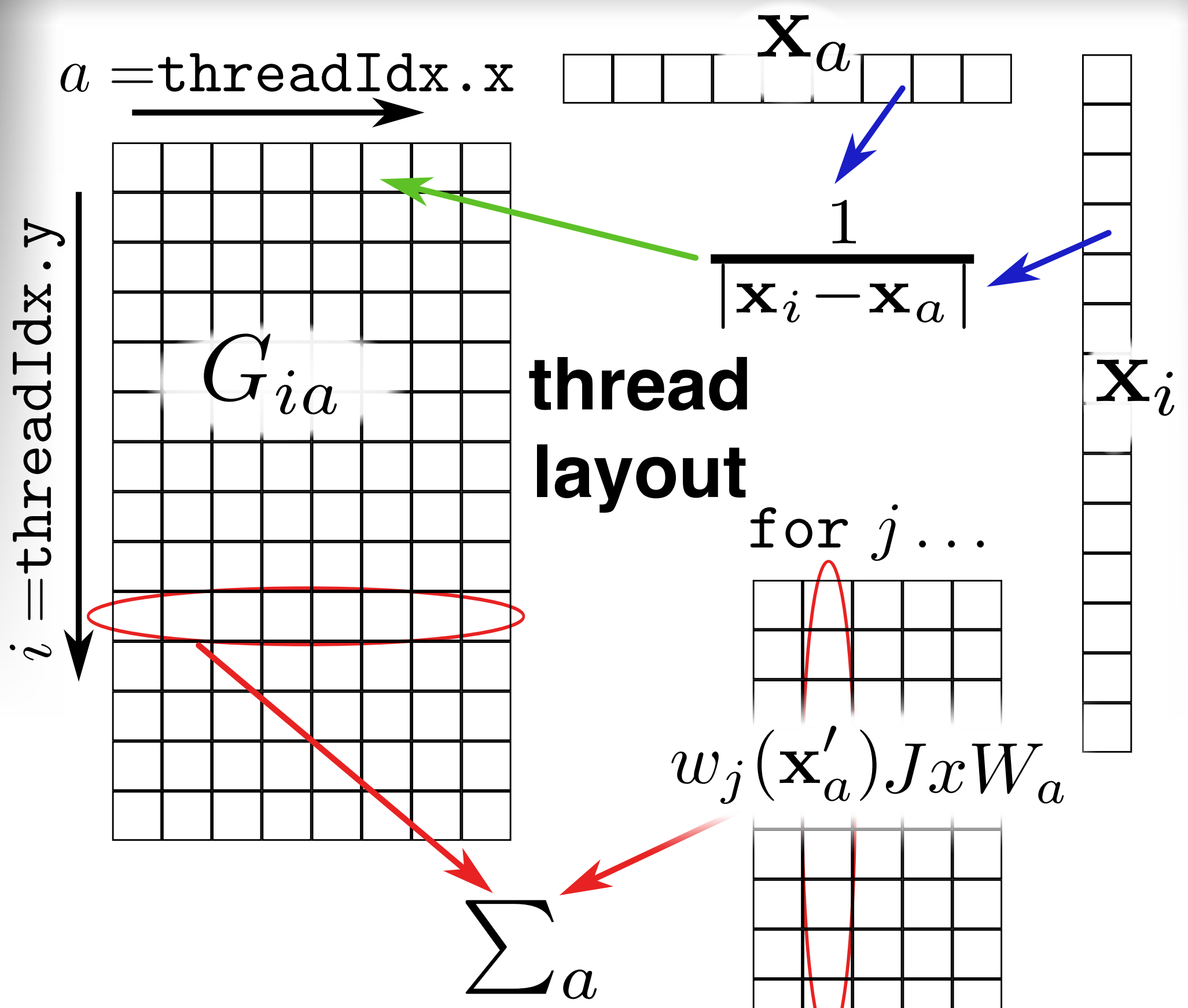


BEM Matrix Assembly with CUDA

Ansatz

$$\Phi = \sum_j \Phi_j w_j$$

$$\frac{\partial\Phi}{\partial\mathbf{n}'} = \sum_j t_j\psi_j$$



Discretized BEM Operators

single-layer
$$V_{h,ij} = \sum_{E\subset S_j}\sum_{a\in E} G_{ia}\psi_{aj}JxW_a\,,$$

double-layer
$$K_{h,ij} = \frac{1}{2}\delta_{ij} - \sum_{E\subset S_j}\sum_{a\in E} H_{ia}w_{aj}JxW_a$$

References

[1] D. Ban et al., 2011. *Kinetics of Conformational Sampling in Ubiquitin.* Angewandte Chemie Int Ed. 2011, 50, 11437 - 11440

[2] S. Kramer, R. Kree, *Single Molecule Impedance Spectroscopy of Proteins by Numerical Simulation,* (in preparation)

[3] S. Kramer PhD Thesis, *CUDA-based Scientific Computing - Tools and Applications,* Universität Göttingen, 2012

[4] C. Holme, *step-28*, CUDA Lab Course 2013

Conclusions

- Assembly of boundary element part implemented with CUDA
- Assembly of finite element part parallelized with QThreads
- CUDA acceleration carries over to individual host thread
- Speedup of **5-8** of hybrid CUDA+QThread implementation (A) over QThread-only (C)