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Compact finite difference formulations for the Poisson equation with application to particle accelerators

Proposal for a bachelor/master thesis

Introduction

The 7-point stencil ∇_7^2 to approximate the Laplacian $-\Delta u(\mathbf{x})$ on a regular grid with spacing h is well known,

$$-\nabla^2 u(\mathbf{x}) = \frac{1}{h^2}\left(6u(\mathbf{x}) - \sum_{j=1,2,3} u(\mathbf{x} \pm h\mathbf{e}_j)\right) + \mathcal{O}(h^2) \equiv -\nabla_7^2 u(\mathbf{x}) + \mathcal{O}(h^2).$$

This stencil is used almost always if the Laplacian is approximated by finite differences for solving, e.g., the Poisson equation, the Navier–Stokes equations, or other equations [2].
The purpose of this thesis is to investigate so-called compact formulations for the Laplacian [4]. One of them is the 19-point stencil

$$-\nabla_{19}^2 u(\mathbf{x}) \equiv \frac{1}{6h^2}\left(24u(\mathbf{x}) - 2\sum_{j=1,2,3} u(\mathbf{x} \pm h\mathbf{e}_j) - \sum_{\substack{j,k=1,2,3\\ j\neq k}} u(\mathbf{x} \pm h\mathbf{e}_j \pm h\mathbf{e}_k)\right).$$

Provided $f(\mathbf{x})$ is sufficiently smooth, a *forth* order finite difference approximation for the Poisson equation $-\Delta u(\mathbf{x}) = f(\mathbf{x})$ is obtained by

$$\nabla_{19}^2 u(\mathbf{x}) = f(\mathbf{x}) + \frac{h^2}{12}\nabla_7^2 f(\mathbf{x}) + \mathcal{O}(h^4).$$

Scope of work

If the work is to become a bachelor thesis the compact formulation is to be incorporated into a (MPI-parallelized) Poisson solver that employs the 7-point stencil so far. If the work is to become a master thesis then additionally the solver is to be integrated into a full-fledged particle solver where a sequence of Poisson problems has to be solved.
Since the compact finite difference formulation is much more accurate than the 7-point stencil, a coarser grid suffices to get the same accuracy in the solution of the Poisson equation. The question is thus: how much coarser can we choose the grid without losing accuracy in the overall solver.
If time permits the compact finite difference formulation is to be incorporated into a solver for non-square domains [1].

Requirements

- Student in computational science or related fields.
- Very good knowledge in numerical mathematics.
- Fluent in C++.
- For the master thesis, attendance in the lecture on "Particle Accereration Methods" by Dr. Adelmann is advantageous.

Deliverables

- The work is to be documented in a short and concise thesis (LaTeX, PDF). It must be written such that it is intelligible to a fellow-student.
- The code should be written as clean as possible. It must be properly documented.
- At the end of the thesis, the work is to be presented in a 30 minutes' talk.

Contact

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- Dr. Andreas Adelmann, Paul Scherrer Institute (PSI), andreas.adelmann@psi.ch

References

[1] A. Adelmann, P. Arbenz, and Y. Ineichen. A fast parallel Poisson solver on irregular domains applied to beam dynamics simulations. *J. Comput. Phys.*, 229(12):4554–4566, 2010.

[2] R. J. LeVeque. *Finite Difference Methods for Ordinary and Partial Differential Equations*. SIAM, Philadelphia, PA, 2007.

[3] S. O. Settle, C. C. Douglas, I. Kim, and D. Sheen. On the derivation of highest-order compact finite difference schemes for the one- and two-dimensional Poisson equation with Dirichlet boundary conditions. *SIAM J. Numer. Anal.*, 51(4):2470–2490, 2013.

[4] W. F. Spotz and G. F. Carey. A high-order compact formulation for the 3D Poisson equation. *Numerical Methods for Partial Differential Equations*, 12(2):235–243, 1996.

[5] K. Zhang, L. Wang, and Y. Zhang. An improved finite-difference method with compact correction term for solving Poisson equations. ePrint archive: `arXiv:1606.07755[math.NA]`, June 2016.

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