Implementing hybrid PDE solvers

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Ευρωπαϊκή Ένωση
Ευρωπαϊκό Κοινωνικό Ταμείο
ΕΠΙΧΕΙΡΗΣΙΑΚΟ ΠΡΟΓΡΑΜΜΑ
ΕΚΠΑΙΔΕΥΣΗ ΚΑΙ ΔΙΑ ΒΙΟΥ ΜΑΘΗΣΗ
επένδυση στην κοινωνία της γνώσης
ΥΠΟΥΡΓΕΙΟ ΠΑΙΔΕΙΑΣ ΚΑΙ ΘΡΗΣΚΕΥΜΑΤΩΝ
ΕΙΔΙΚΗ ΥΠΗΡΕΣΙΑ ΔΙΑΧΕΙΡΙΣΗΣ
ΕΣΠΑ
2007-2013
πρόγραμμα για την ανάπτυξη
ΕΥΡΩΠΑΪΚΟ ΚΟΙΝΩΝΙΚΟ ΤΑΜΕΙΟ
Με τη συγχρηματοδότηση της Ελλάδας και της Ευρωπαϊκής Ένωσης

Outline

Objectives

Overall Objective

Effectively combine

- conventional deterministic PDE solving methods and
- traditional probabilistic Monte Carlo approaches

for solving linear Elliptic Partial Differential Equations.

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Design, implement and evaluate a robust and easy to use prototype system that allows further experimentation in order to elucidate the capabilities and computational characteristics of the resulting PDE solvers.

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Long term goal

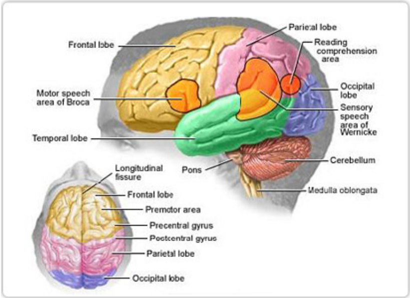
Provide practical (production?) computational tools that add value to existing high performance PDE solvers.

Basic idea

Stochastic pre-processing A Monte Carlo-based walk on spheres approach is utilized to decouple the original PDE problem into a set of independent PDE sub-problems.

Deterministic solving Each of the resulting sub-problems is solved independently by an appropriately selected PDE solver.

Long and short term: PDE problems



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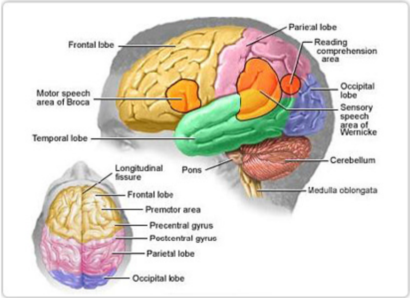

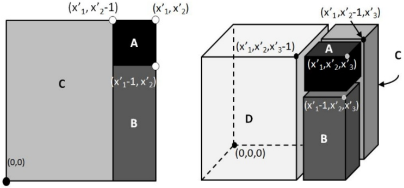

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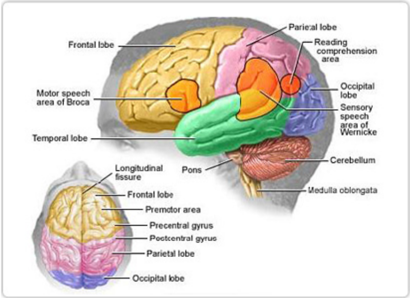

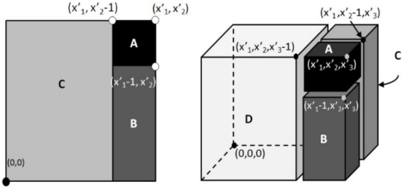

BEWARE:

Specific Algorithm (1/2)

PDE Problem

$$
\begin{aligned}
Lu(x) &= f(x) \quad x \in \mathcal{D} \subset \mathbb{R}^d, \\
Bu(x) &= g(x) \quad x \in \partial\mathcal{D},
\end{aligned}
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PDE Problem

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Subdomains and Interfaces

$$\mathcal{D} = \cup_{\mu=1}^{\mathcal{N}_{\mathcal{D}}} \mathcal{D}_\mu$$
$$\mathcal{I}_{\mu,\nu} = \partial\mathcal{D}_\mu \cap (\partial\mathcal{D}_\nu \cup \mathcal{D}_\nu) \subset \mathbb{R}^{d-1}, \quad \mu \neq \nu, \quad \mu, \nu = 1, \ldots, \mathcal{N}_{\mathcal{D}}.$$

Specific Algorithm (2/2)

Data: $i_1, i_2, \ldots, i_N$: subdomains we wish to compute the solution.
Result: $\tilde{u}_\mu$, $\mu = i_1, \ldots, i_N$: computed solutions in $\mathcal{D}_\mu$

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```
// PHASE I: Estimate solution on interfaces
```

while $\mathcal{I}_{\mu,\nu} \subset \cup_{j=1}^{N} \partial \mathcal{D}_{i_j}$ **do**

  Select control points $x_i \in \mathcal{I}_{\mu,\nu}, \quad i = 1, 2, \dots, M_{\mu,\nu}$;
  Estimate the solution u at x_i by Monte Carlo;
  Calculate the interpolant $u^I_{\mu,\nu}$ of $u_{\mu,\nu}$ using x_i;

end

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`// PHASE II: Compute solution in subdomains`

for $j = 1, 2, \ldots, N$ **do**

Solve the PDE problem:;

$$L_{i_j} u_{i_j}(x) = f_{i_j}(x) \quad x \in \mathcal{D}_{i_j} \; ;$$
$$B_{i_j} u_{i_j}(x) = g_{i_j}(x) \quad x \in \partial\mathcal{D}_{i_j} \cap \partial\mathcal{D} \; ;$$
$$L^*_{i_j} u_{i_j}(x) = h_{i_j}(x) \quad x \in \mathcal{D}_{i_j}$$

end

State-of-the-art

- M. Muller, *Some Continuous Monte Carlo Methods for the Dirichlet Problem*, Annals Mathem Statistics, 1956.
- J. DeLaurentis and L. Romero, *A Monte Carlo method for Poisson's equation*, J. Comput. Phys., 1990.
- M. Mascagni, A. Karaivanova, and Y. Li, *A quasi-Monte Carlo method for elliptic PDEs*. Monte Carlo Methods and Applications, 2001.
- R. Papancheva, I. Dimov, and T. Gurov. *A new class of grid-free Monte Carlo algorithms for elliptic BVP*, Numerical Methods and Applications, 2003.
- J. Acebron, M. Busico, P. Lanucara, and R. Spigler, *Domain decomposition solution of elliptic boundary-value problems via Monte Carlo and quasi-Monte Carlo methods*. SIAM Journal of Sci. Comp., 2006.
- PDD-HPC Research project (Acebron at al.)

Nevertheless

To the best of our knowledge

- No systematic experimentation as been performed.
- No state-of-the-art PDE solving modulus have been considered.
- No practical issues have been raised.
- No software components are readily available.
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Isolated and sporadic efforts.

Basic algorithms and software components

- Our QMC implementations based on known random walks on spheres algorithms. GRID FREE!
- Use of standard C++ library
- Common 2D and 3D user interface
- SINTEF's Multilevel B-splines library for interpolation
- State of the art PDE solvers from http://www.dealii.org/ (2007 J. H. Wilkinson Prize for Numerical Software)
- State of the art graphics integration (TecPlot)

Selected experiments in 2D

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x,y),\ \forall (x,y) \in \Omega \equiv [-1,1] \times [-1,1],$$

$$\left.\begin{aligned} u(\pm 1, y) = &\quad \cosh(\pm 2)\cos(2\pi y) \\ u(x, \pm 1) = &\quad \sin(\pi x)\sinh(\pm 1) + \cosh(2x), \end{aligned}\right. \quad \forall (x,y) \in \partial\Omega.$$

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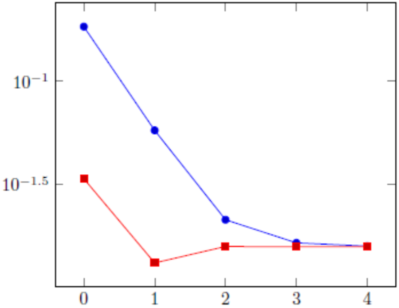
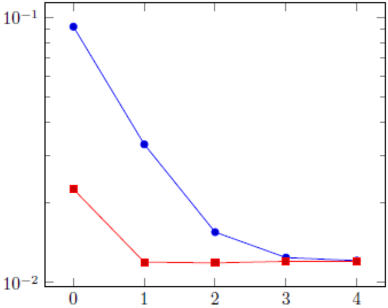
- 8 subdomains with interfaces at $x_1 = 0$, $y_1 = -0.5$, $y_2 = 0$ and $y_3 = 0.75$.
- Seek the solution only in $\Omega_{1,0}$, $\Omega_{0,1}$ and $\Omega_{2,1}$

Error reductions for various configurations





GPU experimentation

- Computing devices:
  - CPU: Intel(R) Core(TM) i7 CPU 870 (2.93GHz)
  - GPU: GeForce GTX 480 (1401MHz)
- Speedups CPU/GPU+CPU
  - Maximum speedup of QMC: 13x
  - Maximum overall speedup: 150x

Trivial implementation!

Web Services experimentation

- Computing servers:
  - Local PCs
  - Tier 3 local computational servers
  - Amazon virtual machines

Low communication/computation ratio

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Synopsis and Prospects

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New line of reasoning that provides new intuition about the dynamics of PDE MC simulations.

https://github.com/mvavalis/Hybrid-numerical-PDE-solvers