

Pozvánka

Katedra mechaniky Fakulty aplikovaných věd
a Výzkumné centrum Nové technologie

si dovoluji pozvat členy akademické obce i odbornou veřejnost na přednášku

Enriched and high-order finite elements for large, accurate ab initio electronic structure calculations

přednáší

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Over the past few decades, the planewave (PW) pseudopotential method has established itself as the dominant method for large, accurate, density-functional calculations in condensed matter. However, due to its global Fourier basis, the PW method suffers from substantial inefficiencies in parallelization and applications involving highly localized states, such as those involving 1st-row or transition-meta atoms, or other atoms at extreme conditions. Modern "real space" approaches, such as finite-difference (FD) and finite-element (FE) methods, can address these deficiencies without sacrificing rigorous, systematic improvability but have until now required much larger bases to attain the required accuracies. In this talk, I'll discuss our recent work on overcoming this critical deficiency of all such real space approaches. In order to substantially decrease basis size (degrees of freedom), one can modify the basis and/or modify the problem. We consider both directions here. First, we discuss a new real-space FE based method [1,2] which employs partition-of-unity FE techniques to substantially increase the efficiency of the representation, thus decreasing degrees of freedom required, by building known atomic physics into the FE basis: without sacrificing locality or systematic improvability. We discuss the weak formulation of the required Kohn-Sham Schroedinger and Poisson problems and the imposition of required boundary conditions. We present both pseudopotential and all-electron applications. Initial results show order-of-magnitude improvements relative to current state-of-the-art PW and adaptive-mesh FE methods for a range of systems having localized states, such as those containing d- and f-electron atoms or other atoms at extreme conditions. Next, we discuss work on a new spectral-element based electronic structure method which decreases required degrees of freedom by a combination of smoothing the problem via a projector-augmented-wave formulation and increasing polynomial order via a well conditioned Lobatto basis. Finally, we highlight recent progress and open questions relating to efficient eigensolvers and parallelization.

[1] N. Sukumar and J.E. Pask, Int. J. Numer. Meth. Eng. 77, 1121 (2009).

[2] J.E. Pask, N. Sukumar, and S.E. Mousavi, arXiv:1004.1765 (2010).

Datum konání: 5. října 2011

Čas konání: 13:00 hod.

Místo konání: místnost 1.75, budova A vědeckotechnologického parku, Teslova 3

Přednáška je pořádána v rámci semináře Fakulty aplikovaných věd (projekt SPAV - CZ.1.07/2.3.00/09.0050)



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