Solving Nonlinear Virus Replication PDE Models With Hierarchical Grid Distribution Based GMG

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Realistic biophysical models in general only can be evaluated by applying advanced numerical solution techniques. The recent COVID19 pandemics has unveiled the need for detailed biophysical understanding of virus replication mechanisms. We are building a framework to mirror intracellular virus replication dynamics by means of fully spatio-temporal resolved PDE models. The models couple effects which are restricted to intracellular 3D embedded 2D curved manifolds with the full 3D intracellular space dynamics. Technically, surface PDEs (sufPDE) are coupled with PDE by the aid of boundary conditions for the PDEs which are reflected by reaction terms of the sufPDEs. The highly nonlinear sufPDE/PDE system is discretized with vertex centered Finite Volumes (vcFV) upon unstructured grids which are reconstructed from experimental data. This study describes the properties of the application of a hierarchical grid distribution based Geometric Multigrid Solver (GMG) to the system of linear equations (SLE) established by a nonlinear Newton solver. We demonstrate the precision and efficient weak scaling up to about 300 Millions degrees of freedom (DoFs) at grid refinement level 4 based on the massively parallel GMG solver implemented in UG4. The biophysical output data demonstrate quantitative consistence with the experimental findings, prompting further advanced experimental studies to validate the model and refine our quantitative biophysical understanding. Our framework allows for realistic intracellular virus replication simulations paving new ways for the development of direct antiviral agents and potent vaccines.

References:

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