NSTRF PROGRESS REPORT – Grant Year 2 PR 4 **NASA Grant Number NNX16AM58H** 7/31/2018 Prediction and Optimization of Truss Performance for Lightweight, Intelligent Packaging and Deployable Structures California Institute of Technology	
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1. GOAL

Create an efficient computational tool capable of predicting the complex, nonlinear response of truss lattices containing extremely large numbers of beams and nodes.

2. MOST SIGNIFICANT TECHNICAL ACHIEVEMENT(S)

Performed my visiting technologist experience at Sandia National Labs in Livermore, California working on the Schwarz Alternating Method for multiscale problems. Extended the existing Schwarz theory for quasistatic problems to work for dynamic problems. Tested the method in a small Matlab code and large high performance finite element code, Albany, to test and improve the performance of the existing implementation, and suggested future work to improve performance further.

3. ACTIVITIES AND ACCOMPLISHMENTS

The Schwarz Alternating Method (subsequently referred to as Schwarz) is a technique that was originally developed to compute the solution to the Poisson equation in irregularly shaped domains, but was later extended to work for more general elliptic partial differential equations, and is largely used as a preconditioner for iterative linear solvers. However, more recently, a team at Sandia has extended the Schwarz theory to show that it can work for nonlinear PDEs, including those of hyperelasticity (REFERENCE).

The equations for hyperelastic solid mechanics can be derived from minimizing the total potential energy of the system

$$\Phi[\boldsymbol{\varphi}] \coloneqq \int_{\Omega} A(\boldsymbol{F})\,dV - \int_{\Omega} R\boldsymbol{B}\cdot\boldsymbol{\varphi}\;dV - \int_{\partial\Omega_2} \boldsymbol{T}\cdot\boldsymbol{\varphi}\,dS$$

over all functions in $H^1(\Omega)$ that satisfy the essential boundary conditions, where $\boldsymbol{F} = \boldsymbol{\nabla}\boldsymbol{\varphi}$ is the deformation gradient, $\boldsymbol{B}$ is the body force, and $\boldsymbol{T}$ is the prescribed traction on the boundary. The proof in the paper makes the assumption that the functional $\Phi[\boldsymbol{\varphi}]$ is strictly convex. Furthermore, the proof relies on the fact that during the Schwarz iterations, the deformation mapping in one Schwarz domain can be naturally extended to the entire domain using the deformation mapping in the remaining fields. For example, in a two-domain Schwarz iteration, the deformation mapping of the entire domain can be written as

$$\boldsymbol{\varphi}(\boldsymbol{X}) = \begin{Bmatrix} \boldsymbol{\varphi_1}(\boldsymbol{X}) & if\ \boldsymbol{X} \in \Omega_1 \\ \boldsymbol{\varphi_2}(\boldsymbol{X}) & if\ \boldsymbol{X} \in \Omega_2 \backslash \Omega_1 \end{Bmatrix} \in H^1(\Omega)$$

where Ω_1 and Ω_2 are the two Schwarz domains.

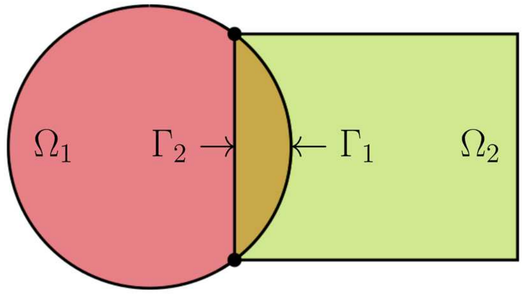

Figure 1. An Example of overlapping Schwarz regions. (REFERENCE)

While this is true in the continuous case, this cannot always be done in the discrete case. For example, if the two discretizations of Ω_1 and Ω_2 (denoted by S_1^h and S_2^h respectively) are non-conforming, writing the deformation mapping in this manner does not result in a conforming mapping, meaning the function is not in $H^1(\Omega)$ and is not admissible. However, this detail is disregarded in the actual implementation and use of the Schwarz method, as the non-conforming error is assumed to be negligible. However, if S_1^h and S_2^h are conforming discretizations (i.e. $S_1^h \cup S_2^h = S^h \subset H^1(\Omega)$) then the extension of the deformation mapping from one Schwarz domain to the entire body is valid.

Even though the proof was done with the intention of applying this to quasistatic hyperelasticity problems, it is really a proof of the Schwarz method for general convex functionals. It is well known that viscoplasticity and dynamics can be formulated in a variational framework using an incremental potential of the form:

$$\Phi^n\left[\boldsymbol{\varphi}^{(n+1)}, \boldsymbol{Z}^{(n+1)}\right] \coloneqq$$
$$\int_\Omega A\left(\boldsymbol{F}^{(n+1)}, \boldsymbol{Z}^{(n+1)}\right) - R\boldsymbol{B}\cdot\boldsymbol{\varphi}^{(n+1)} + D\left(\boldsymbol{Z}^{(n+1)}, \boldsymbol{Z}^{(n)}\right) + K\left(\boldsymbol{\varphi}^{(n+1)}, \boldsymbol{\varphi}^{(n)}, \dot{\boldsymbol{\varphi}}^{(n)}\right) dV$$
$$- \int_{\partial\Omega_2} \boldsymbol{T}\cdot\boldsymbol{\varphi}^{(n+1)}\, dS$$

where $\boldsymbol{Z}$ are the internal variables, D is the incremental dissipation potential, K is the potential associated with the variational integrator, and the superscripts (n) and (n+1) denote the variables at the current and next time step respectively. Another way of writing the potential is as a sum of potentials

$$\Phi^n\left[\boldsymbol{\varphi}^{(n+1)}, \boldsymbol{Z}^{(n+1)}\right] \coloneqq \Phi\left[\boldsymbol{\varphi}^{(n+1)}\right] + D\left(\boldsymbol{Z}^{(n+1)}\right) + K\left(\boldsymbol{\varphi}^{(n+1)}\right)$$

Given that the hyperelastic, dissipation, and dynamic potentials are convex, the resulting incremental potential is also convex. Assuming that the hyperelastic potential is convex (this is assumed for the quasistatic case already) and the dissipation potential is convex (which is a reasonable assumption), the only thing left to show is the dynamic incremental potential is convex. For the case of the energy-preserving Newmark integrator (with $\gamma = 1/2$), the incremental potential can be written as

$$K\left(\boldsymbol{\varphi}^{(\boldsymbol{n+1})}\right) = \frac{-1}{2\beta\Delta t^2}\int_{\Omega} \rho \left(\boldsymbol{\varphi}^{(\boldsymbol{n+1})} - \left(\boldsymbol{\varphi}^{(\boldsymbol{n})} + \Delta t \dot{\boldsymbol{\varphi}}^{(n)} + (1-2\beta)\ddot{\boldsymbol{\varphi}}^{(n)}\right)\right)^2 dV$$

with the usual Newmark update formulas for $\dot{\boldsymbol{\varphi}}^{(n)}$ and $\ddot{\boldsymbol{\varphi}}^{(n)}$. This is quadratic in $\boldsymbol{\varphi}^{(\boldsymbol{n+1})}$, so it is clearly a convex function of $\boldsymbol{\varphi}^{(\boldsymbol{n+1})}$.

Just as it was desirable to use non-conforming discretizations in each Schwarz domain, it is desirable to use different time steps or different time integrators in each Schwarz domain. The theory outline above does not guarantee convergence or accuracy of using different time steps or different integrators in different domains, as the incremental functional depends on the integrator and time step, but some 1D test cases show that this can be done is certain cases without the introduction of significant error.

In order to test the Schwarz method for dynamic problems, I simulated a dynamic tension pull test on an Aluminum dog-bone specimen. The Aluminum was modeled using a finite deformation J2 plasticity model based on (REFERENCE). The Newmark integrator with $\beta = 1/4$ and $\gamma = 1/2$ was in both domains. The gauge section of the specimen was modeled using composite 10-node tetrahedral elements (REFERENCE), while the ends were meshed with hexahedral elements.

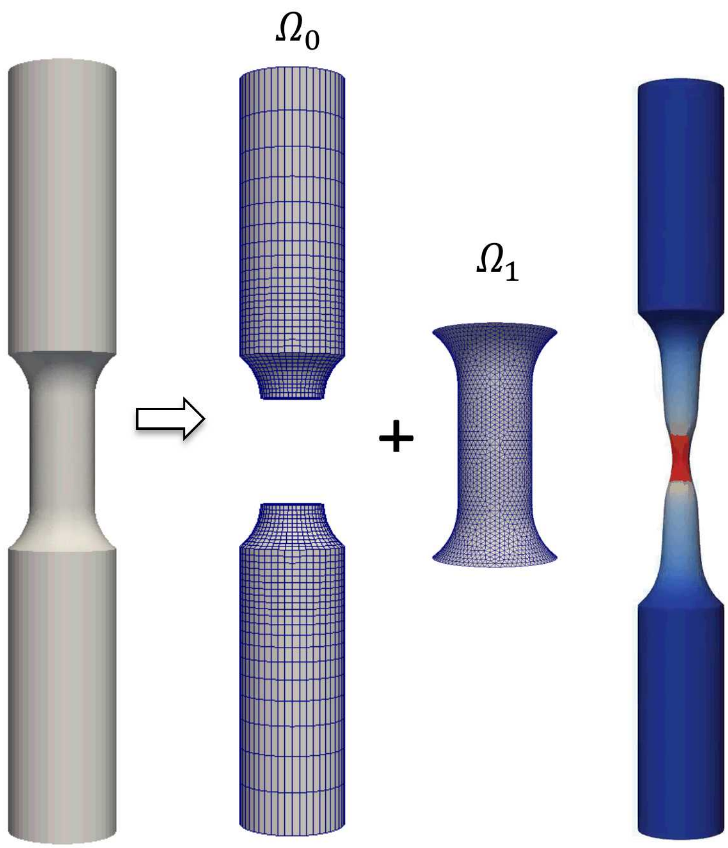

Figure 2. Tension specimen decomposed into the two Schwarz domains meshed with hexahedral and tetrahedral elements (left) and the equivalent plastic strain of the pulled tension specimen (right).

The tension specimen was pulled such that the gauge section exhibited necking (see Figure 2). The simulation was performed using the Schwarz method outlined above and with a standard single-domain method. Both methods showed excellent agreement, suggesting that the Schwarz method did not introduce any significant errors

4. PLANNED ACTIVITIES

Over the next quarter, I will resume work on the TrussQC method and focus on using higher order interpolation and new energy summation techniques to reduce the locking phenomena seen in previous fracture toughness simulations. This will require using new mesh data structures and meshing techniques to create higher order triangle and tetrahedral elements.

5. VISITING TECHNOLOGIST EXPERIENCE(S)

COMPLETED Visiting Technologist Experience			
Start Date	***End Date***	***NASA Center or R&D Lab***	***Activities and Relevance to Research Goals***
06/19/2017	08/25/2017	JPL	This project will focus on performing experiments on a variety of lattice samples to investigate how the microstructure affects the fracture toughness of the macroscopic material. The constituent material, relative density, and the unit cell topology will be varied between samples. Results will be compared with existing theory for fracture mechanics of lattice materials and computational simulations. These experiments will help with the validation of TrussQC.
PLANNED Visiting Technologist Experience			
Start Date	***End Date***	***NASA Center or R&D Lab***	***Activities and Relevance to Research Goals***
5/1/2018	8/3/2018	Sandia National Labs	I will work on multiscale modeling of dynamic problems using the Alternating Schwarz Method. I will work on some theory and also implementation and testing of the method using Sandia' finite element code, Albany.

6. ISSUES / CONCERNS

N/A

7. REFERENCES

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