

Peridynamic Modeling of the Kalthoff-Winkler Experiment

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Abstract

The peridynamic model is a new theory of continuum mechanics that is specifically oriented toward modeling problems in which cracks or other discontinuities emerge spontaneously as a body deforms under load. In this study, the code that implements this theory, EMU, is applied to a dynamic single-fracture experiment in a tough steel specimen. Accuracy of the method is illustrated by comparison with experimental data. Scaling properties of the code on C-plant are investigated, including dependence of speedup on the material model used. Excellent scaling properties are obtained with a material model that has low requirements for memory and communications.

1. Introduction

Many problems of fundamental importance in mechanics involve the spontaneous emergence of discontinuities, such as cracks, in the interior of a body. The classical theory of continuum mechanics is in some ways poorly suited to modeling this type of problem, because the theory uses partial differential equations as a mathematical description. The required spatial derivatives, by definition, do not exist on the surfaces of discontinuity, so the entire formulation breaks down when such discontinuities form. Although much work has been devoted to special techniques aimed at working around this problem, particularly in the theory of fracture mechanics, these techniques are not fully satisfactory either in principle or in practice as general descriptions of fracture. This difficulty is inherited by numerical methods that implement the classical theory, including nearly all finite-element and finite-difference codes in common usage at Sandia and elsewhere.

Although this problem may appear at first glance as merely an academic issue, this inapplicability of the theory to discontinuities severely limits our ability to numerically model cracks, shock waves, shear bands, phase boundaries, and many other phenomena. These features are of critical importance to Sandia's responsibility for modeling material deformation and structural failure in nuclear weapons and other applications.

For this reason, Sandia has been developing a new theory of continuum mechanics, known as the *peridynamic* model [1]. This model avoids the fundamental mathematical difficulty by using integral equations as a description of material motion rather than differential equations. Therefore, the presence of discontinuities in a deforming body does not limit the applicability of the peridynamic theory.

A computer code called EMU that implements the peridynamic theory is currently under development. The code is showing promise in the modeling of penetration and impact problems where the discrete nature of fracture is important. An example of such an application is perforation of thin ductile plates, in which the load on the penetrator is strongly influenced by the formation of a few radial cracks that separate the target into "petals." The EMU simulation of this problem is shown in Figure 1.

Because the formulation is oriented toward modeling cracks and other discontinuities, it is important to carry out validation of EMU against data from single-crack dynamic fracture experiments. The purpose of the current exercise is to provide validation of EMU with respect to dynamic fracture and to demonstrate its performance on a massively parallel computer.

2. Peridynamic theory

As remarked above, the peridynamic theory replaces the basic equations of the classical theory of continuum mechanics. The equation of motion in the peridynamic theory is

$$\rho \ddot{u} = \mathcal{L}_u + b$$

where ρ is mass density, u is the displacement vector field, b is the body force density, and \mathcal{L}_u is a functional of displacement. There are many possible choices for \mathcal{L}_u . The most intuitive and most widely studied is as follows:

$$\mathcal{L}_u(\tilde{x}, t) = \int_R \tilde{f}(u(\tilde{x}', t) - u(\tilde{x}, t), \tilde{x}' - \tilde{x}) dV_{\tilde{x}'}$$

where \tilde{f} is a vector-valued function. Note that here \tilde{x} is the point where acceleration is being evaluated while \tilde{x}' is the dummy variable of integration (Figure 2). The physical interaction between \tilde{x} and \tilde{x}' is referred to as a *bond*.

The function \tilde{f} contains all the constitutive information about the material. It represents the force per unit volume that \tilde{x}' exerts on \tilde{x} due to the bond between these points. Note the resemblance between the current formulation and molecular dynamics (MD) due to the summation of forces between particles separated by a finite distance. However, the peridynamic theory is also fundamentally different from MD in that the peridynamic model is truly a continuum theory and is not restricted in size scale to the atomic level.

It is convenient and reasonable to assume that material particles separated by a distance greater than some fixed number δ do not interact. This number is called the *horizon* for the material.

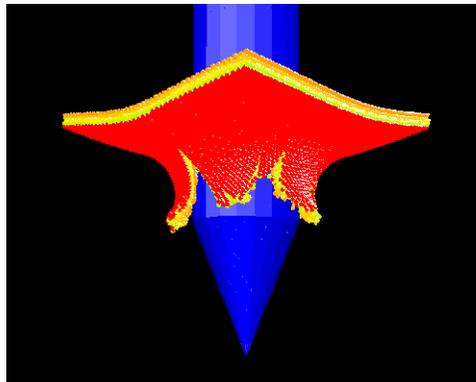


Figure 1. Typical EMU application: petaling during perforation of a thin ductile plate.

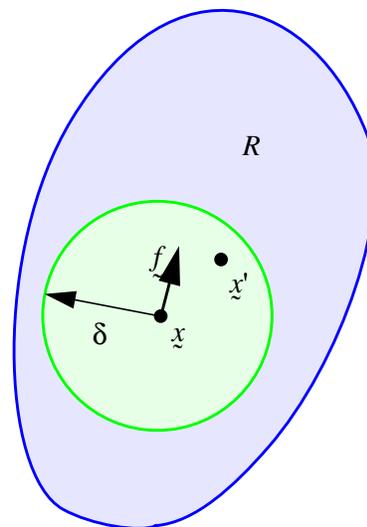


Figure 2. Schematic of variables used in evaluation of \mathcal{L}_u .

3. Numerical method

EMU evaluates the integral in L_u using the “brute force” approach illustrated in Figure 3. The acceleration of node i is being evaluated, and the integration occurs over all nodes j located within a distance δ from node i . The acceleration is found from the discretized form of L_u :

$$\rho \ddot{u}^i = \sum_{|x^j - x^i| < \delta} f(u^j - u^i, x^j - x^i)(\Delta x)^3$$

Integration in time is performed using explicit central differencing.

Figure 3 illustrates a rectangular structured grid, but extension to nonrectangular or nonstructured grids is straightforward.

The method described above is “brute force” in the sense that it does not take advantage of more efficient means of evaluating integrals such as octree or multigrid techniques. More sophisticated methods will be examined for future EMU development.

Parallelization is performed by allowing each processor to be responsible for a fixed region of space (Figure 4). As the body deforms, nodes are permitted to migrate between processors. After each time step, the updated variables for nodes within a distance δ of a given processor are passed to that processor to be used in the following cycle.

This parallelization technique has the advantage of simplicity and works well for applications in which the motion of the nodes is not too large. More sophisticated load balancing methods will be considered as part of future development of EMU to account for possible large displacements.

4. Kalthoff-Winkler problem description

A well-known dynamic single-fracture experiment is the *Kalthoff-Winkler* experiment [2]. In this experiment, a plate of tough maraging steel has two parallel notches cut into it with circular tips (Figure 5). A steel impactor strikes the plate edge-on.

The plate material is X2 NiCoMo 18 9 5. This is apparently similar to Standard Grade 18Ni(300). The composition is 18% nickel, 9% cobalt, and 5% molybdenum. According to handbook data [3], the tensile

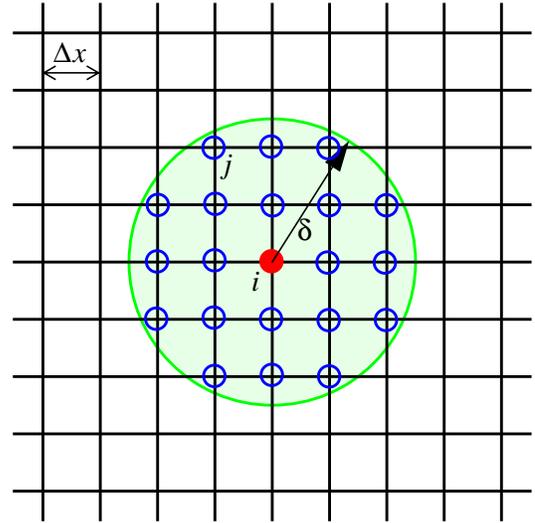


Figure 3. Nodes contributing to the acceleration of node i .

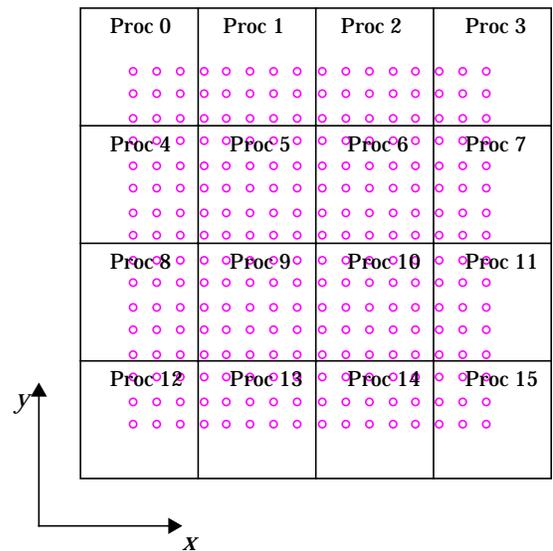


Figure 4. Regions of space owned by the processors and typical nodes within these regions. Nodes can migrate between processors as the grid deforms.

strength of this material is about 2000 MPa and the fracture toughness is about $90 \text{ MPa}\cdot\text{m}^{1/2}$. The plate mass density was assumed to be 8000 kg/m^3 .

The impact creates compressive stress waves that move into the interior of the plate. As these waves interact with the notch tips, mode-II loading occurs. Depending on the impact velocity, fracture may initiate at the notch tips. Surprisingly, in these cases, the cracks do not grow parallel to the notches. Instead, they grow at 68 degree angles to the notches. The ability of a code to reproduce this angle is a sensitive test of whether it can model fracture accurately. (Certain choices of impact velocity were found in the experiment to lead to the formation of shear bands rather than cracks.)

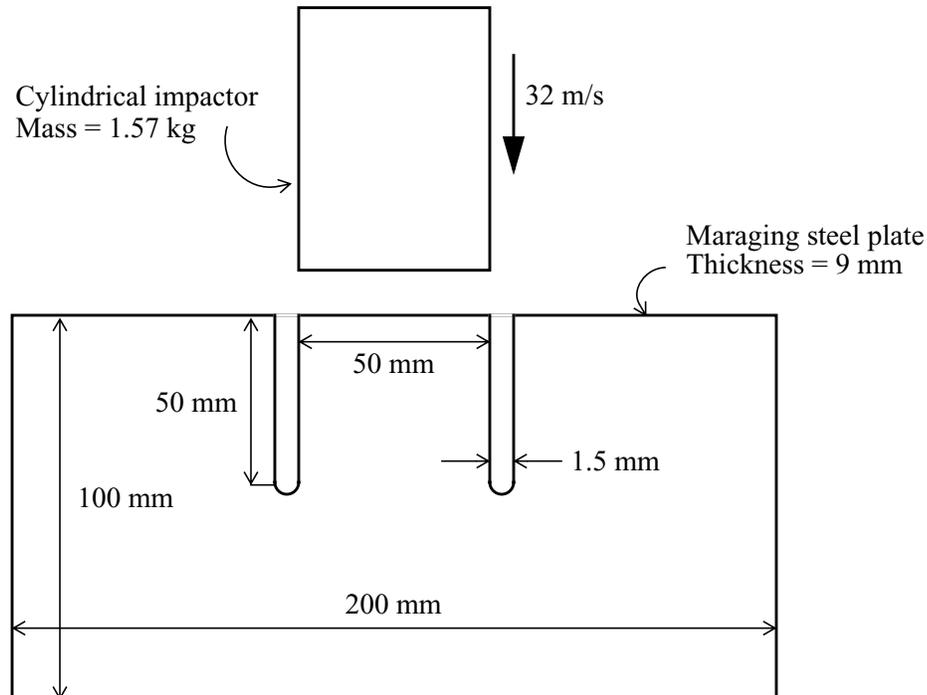


Figure 5. Experimental setup (notches are not drawn to scale).

5. Computational model

The EMU model used a rectangular, equally spaced structured grid with dimensions $200 \times 100 \times 9$. The impactor was assumed to be a rigid cylinder. The grid boundaries were load-free all around.

Two different material models were used in this study. These are illustrated in Figure 6, which shows plots of bond stretch between two arbitrary nodes and bond force per unit volume. The first model, called *microelastic*, loads along the path shown. The bond breaks if its stretch reaches a critical value ϵ_0 . If the bond breaks, it stays broken forever, and the force in the bond remains zero. If it does not break, unloading occurs along the original loading path.

The second material model considered is called *microplastic*. This is similar to the microelastic model, except that unloading occurs along the path shown (if the bond does not break first), leading to a permanent stretch in the bond upon full unloading.

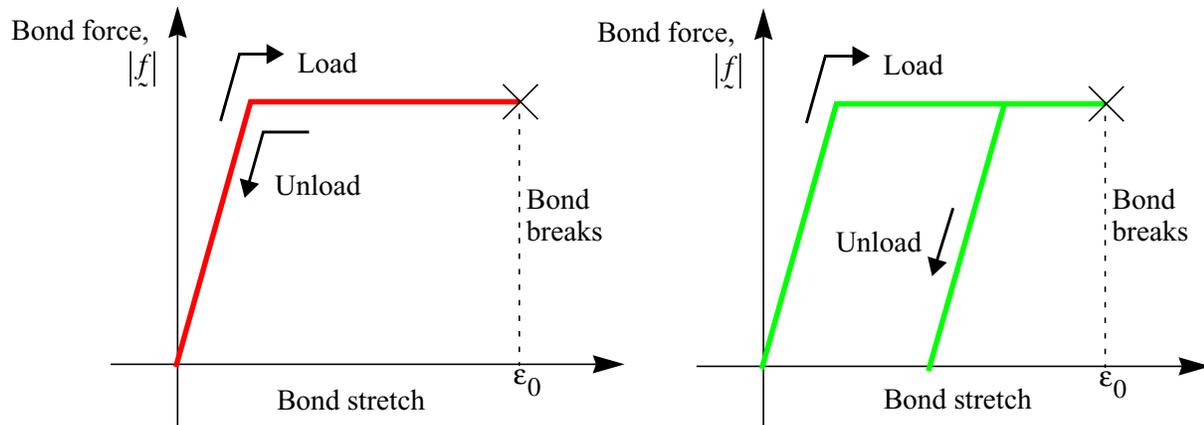


Figure 6. Loading and unloading paths for a single bond in the microelastic (left) and microplastic (right) material models. In either model the bond can break irreversibly.

These two material models, although they give similar results in most applications, differ widely in their computational requirements. The reason is that the microplastic model requires the storage of current bond stretch values for each node j that interacts with a given node i . Since typically $\delta = 3\Delta x$, where Δx is the mesh spacing, this means that approximately 113 ($\approx 4\pi^3/3$) variables must be stored for each node in the microplastic model, and these variables must be passed between processors along with the other variables. So, the implications of the two material models for massively parallel implementation are quite different.

For the EMU model of the Kalthoff-Winkler experiment, the material parameters corresponded to a Young's modulus of 191 GPa, a Poisson ratio of 0.3, a mass density of 8000 kg/m³, a fracture toughness of 90 MPa-m^{1/2}, and a tensile strength of 2000 MPa.

6. Results

Figure 7 shows the initial and final configurations of the body. The code correctly predicts the experimentally observed crack angle and the fact that the cracks propagate all the way to the free surfaces. These results are shown in Figure 8 for both material models. The crack length as a function of time is shown for both materials in Figure 9. The similarity between the two curves indicates that physically, the material models are behaving nearly identically.

A view of the cracks while they are growing is given in Figure 10, which shows synthesized Moire fringes. Each fringe has constant displacement in the y direction, which is parallel to the notches. In this figure, the displacements are exaggerated by a factor of 10 to make the crack shapes more visible.

7. Code performance

The EMU model with 180,000 nodes was run for 700 time steps on the Alaska C-plant with both material models. The runtimes (wall clock times) are illustrated in Figure 11. Ideal linear speedup would correspond to a straight line with slope -1 as indicated. Evidently the microelastic model comes closer to this ideal than the microplastic model. This difference is due to the more burdensome message passing requirements of the microplastic model, as discussed above. With the microelastic model, scaling is fairly close to linear over the range measured. However, it is likely that a minimum in this runtime curve exists somewhere to the right of the range shown (the microplastic curve shows signs of approaching such a mini-

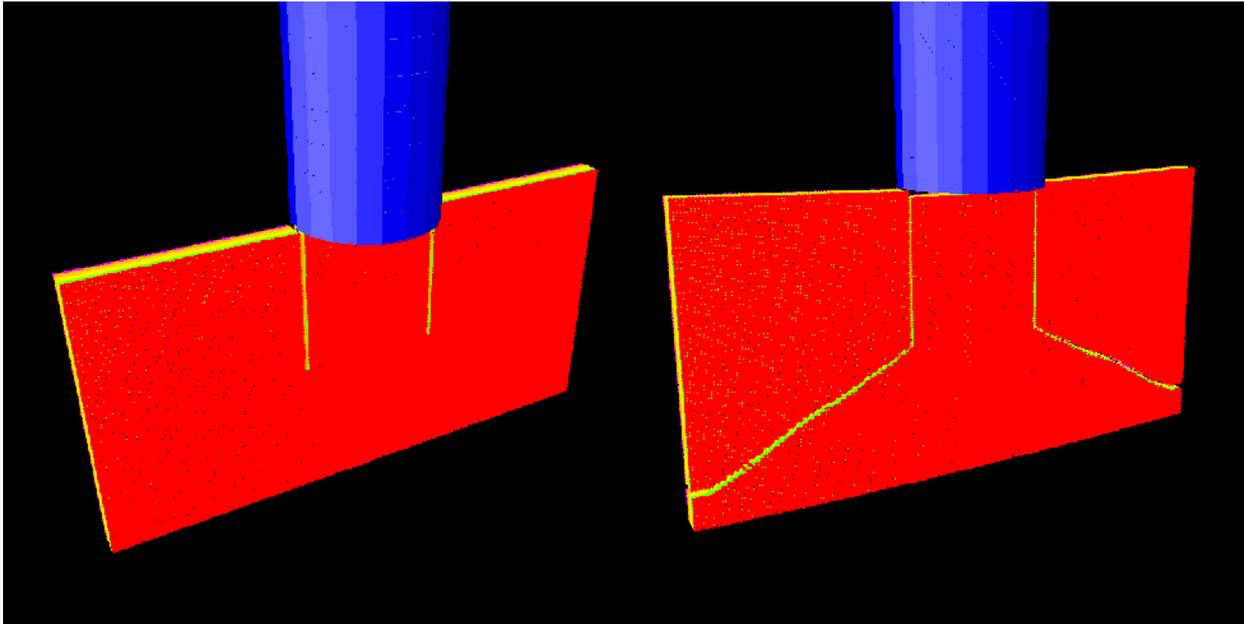


Figure 7. EMU mesh and rigid impactor. Left: initial. Right: final.

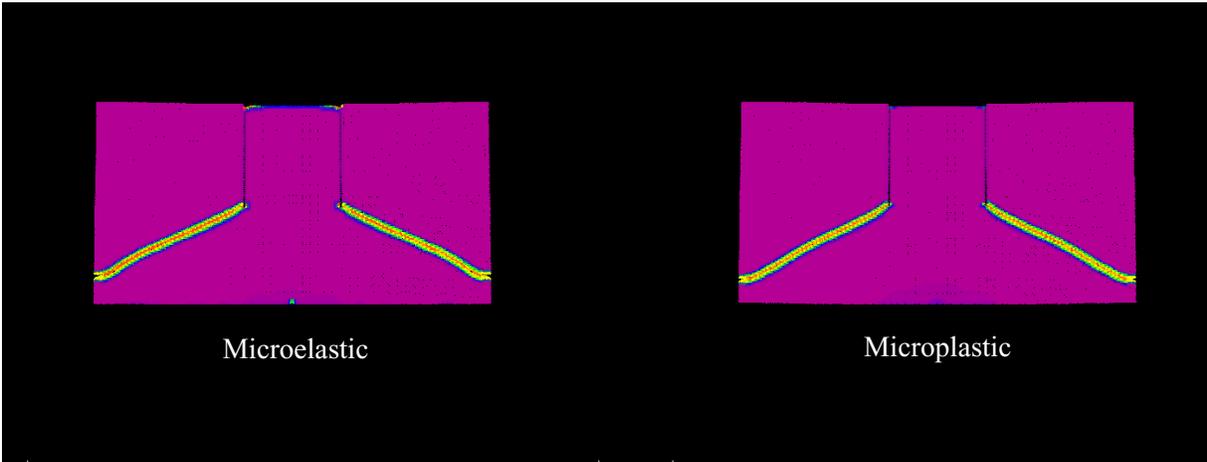


Figure 8. Crack paths (shown as contours of damage) predicted by EMU for both material models.

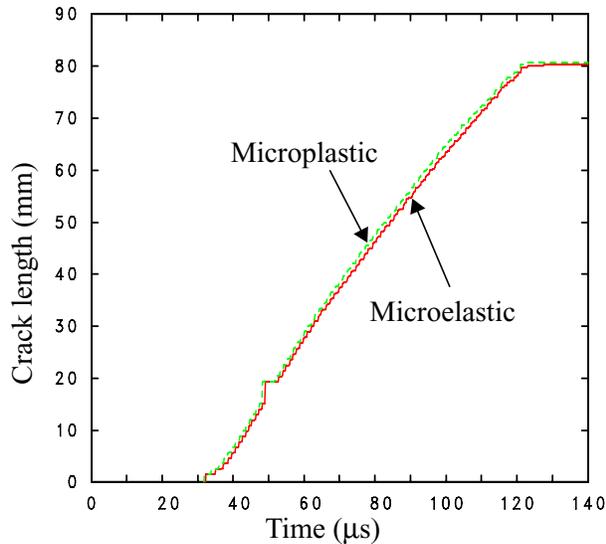


Figure 9. Crack length (measured from the original notch tip location) as a function of time for both materials.

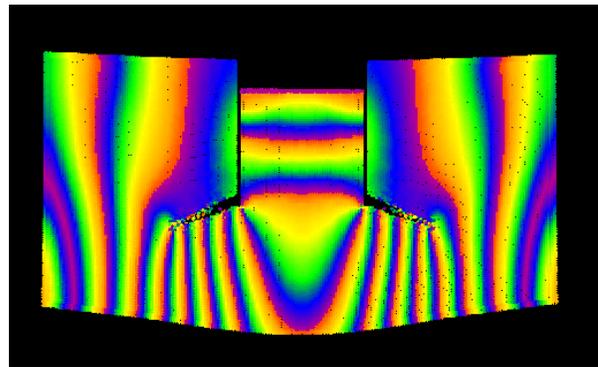


Figure 10. Synthesized Moire fringes showing crack shapes at time 60 μ s. Displacements are exaggerated.

mum). A minimum in the microelastic curve is expected because in the limit of one node per processor, variables for each node would need to be passed to the processor for every other node in its horizon in each time step, which is clearly an inefficient process.

8. Conclusions

As a standard problem in dynamic fracture mechanics, this successful simulation of the Kalthoff-Winkler problem represents an important milestone in the development and validation of the peridynamic theory. Because this technique does not require the specification of kinetic laws for crack growth, and because it does not require the tracking of individual cracks, it models fracture mechanics problems of arbitrary complexity with potentially great generality. The Sandia applications of this technique are immediate and include penetration mechanics and a wide range of problems involving material failure.

From a computational point of view, the main difference between EMU and standard hydrocodes is that in EMU, each node interacts with many other nodes, not just with its nearest neighbors. This property, which arises from the use of the underlying integral equation formulation, influences the picture of what an optimum massively parallel system would look like for running the code.

The performance of the code on C-plant is shown in this study to depend on the material model. The microelastic model, which does not require the storage of significant amounts of bond data, scales very well as the number of processors is increased, as shown in Figure 11. With this material model, the code is essentially compute limited unless the number of processors is very large. When the microplastic model is used, more communication time between processors is required because of the greater quantity of bond data used in the model. Therefore, in this case, the code tends to be limited by communication speed and memory. This leads to less impressive, although still acceptable, scaling properties of the microplastic model on C-plant compared with the microelastic model.

Note that the vast majority of Sandia applications, especially penetration and impact calculations, are expected to require only the simpler microelastic model. In this case the current C-plant architecture is

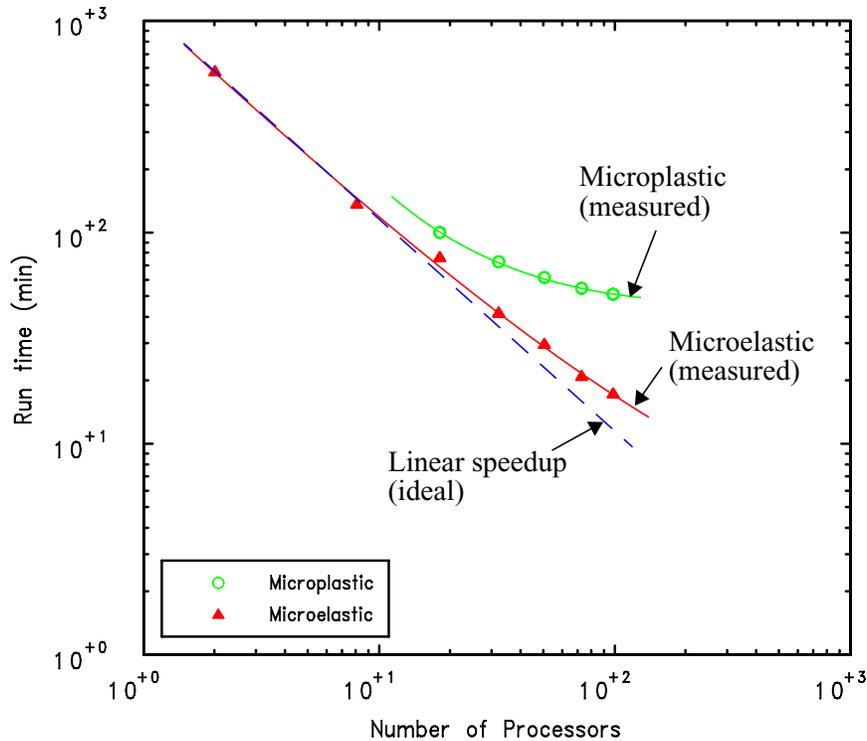


Figure 11. Runtimes on Alaska C-plant for both material models with the 180,000 node grid for the Kalthoff-Winkler model. The dashed line shows the ideal case of linear speedup (slope = -1). The microplastic model cannot be run with fewer than 18 processors because of memory requirements.

close to ideal. However, problems in which cyclic loading is important, such as fatigue cracking, might require the microplastic model. For such problems, the present study shows that improvements in communication speed and memory per processor would have a favorable impact on the runtimes. The same situation applies to problems involving true long-range forces such as Van der Waals interactions, in which case the horizon might be large compared with the mesh spacing. For such problems, more sophisticated integration methods such as multigrid could potentially cut down on the communications requirements.

In spite of these considerations, this study has shown that EMU yields accurate results on an important validation problem, and that the numerical method can make effective use of the C-plant architecture.

References

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