

PSD: Parallel Finite Element Solver for Continuum Dynamics

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Summary

PSD (Parallel finite element Solver for continuum Dynamics) is an open-source finite element method (FEM) solver designed for high-performance computing simulations in continuum dynamics with a special focus on earthquake mechanics. It enables integrated fault-to-site seismic simulations by combining advanced material modeling, scalable parallelism, and purpose-built meshing-partitioning tools.

Built on FreeFEM (Hecht, 2012) for FEM discretization and PETSc (Balay et al., 2019) for scalable linear solvers, PSD integrates non-linear material modeling through its MFronT (Helfer et al., 2015) interface for realistic simulations. Its custom MPI I/O-based mesher-partitioner, top-ii-vol (Badri et al., 2024), enables efficient on-the-fly mesh generation and partitioning for earthquake geometries, removing sequential meshing bottlenecks. On the structural side, hybrid phase-field fracture mechanics (Ambati et al., 2015) for crack analysis is implemented. This spans the full simulation chain from earthquake source to structural assessment.

A key feature of PSD is its ability to perform fault-to-site earthquake simulations with billions of degrees of freedom, scaling efficiently on tens of thousands of MPI-processes, making it suitable for comprehensive seismic risk assessment.

Statement of Need

Seismic risk assessment requires tools that can simulate wave propagation across multiple scales, from faults (kilometers away) to local site response (meters), with sufficient accuracy. Commercial software often lacks the scalability needed for regional simulations, while open-source alternatives typically focus on specific parts of the seismic workflow.

Current computational challenges in earthquake simulation include: (1) handling billions of degrees-of-freedom to capture realistic fault-to-site scenarios (Hori et al., 2018), (Cui et al., 2013), (2) integrating complex non-linear material behaviors and damage assessment for solids and structures, and (3) efficiently generating and partitioning large meshes for irregular geological domains derived from digital elevation models. FEM tools like OpenSees (McKenna, 2011) excel in local-site response, while SPEC3D (Peter et al., 2011) and SEM3D (Touhami et al., 2022) address wave propagation using spectral elements. An open-source platform covering the full fault-to-site workflow with HPC scalability remains highly desirable.

PSD tries to fill this gap by providing a unified framework that combines earthquake wave propagation simulation and structural mechanics assessment within a single scalable FEM solver. PSD's integration of advanced meshing-partitioning capabilities, sophisticated material modeling, and fracture mechanics positions it uniquely for comprehensive seismic risk assessment needs

41 requiring both regional-scale wave propagation and local site response, including structural
42 analysis.

43 Features and Architecture

44 PSD offers a range of physics modules designed for earthquake simulations, including linear
45 elasticity, elastodynamics, fracture mechanics, soildynamics¹, and elasto-plasticity. Its versatility
46 is further enhanced by the Mfront interface, which allows users to implement custom non-linear
47 material models, that can be seamlessly integrated into any of these modules expanding their
48 capabilities beyond its built-in constitutive laws. Additionally, comprehensive verification and
49 validation campaigns for all PSD modules, with results cross-compared against reference codes,
50 experimental data, and analytical benchmarks, ensuring transparency and reproducibility (see
51 [validation page](#)).

52 PSD adopts a layered architecture that separates mathematical formulation from computational
53 implementation while maintaining high performance through strategic integration. It follows
54 a code generation approach where users specify problem configurations through command-
55 line options, and the it automatically generates optimized code tailored to specific physics,
56 dimensionality, and boundary conditions. This design enables computational efficiency while
57 preserving flexibility for diverse applications across the available physics modules.

58 The parallel computing architecture in PSD employs domain decomposition strategies that
59 enable distributed memory parallelization which are optimized for large-scale FEM simulation
60 (Dolean et al., 2015). PSD has demonstrated scalability up to 24,000 cores and capability for
61 handling problems with over 5 billion unknowns for earthquakes.

62 Example Workflow

63 A representative application illustrates PSD's soildynamics module for 3D wave propagation
64 in an elastic domain with paraxial absorbing boundaries (Modaressi & Benzenati, 1994) and
65 double-couple point sources (Benz & Smith, 1987). This example illustrates one of PSD's
66 specialized physics modules, among others. The aim here is to briefly illustrate PSD's key
67 capabilities, including automated distributed mesh generation, advanced time integration, and
68 sophisticated boundary condition handling.

69 **Mathematical Presentation:** PSD solves the elastodynamic wave equation using FEM discretiza-
70 tion with Newmark- β time integration. For a domain $\Omega \subset \mathbb{R}^3$ and with paraxial absorbing
71 boundaries $\partial\Omega_p \subset \partial\Omega$, the FEM weak form reads:

Find $\mathbf{u} \in \mathcal{U}$ such that $\forall t \in [0, t_{\max}], \forall \mathbf{v} \in \mathcal{V}$:

$$\begin{aligned} & \int_{\Omega} \left(\frac{\rho}{\beta \Delta t^2} \mathbf{u} \cdot \mathbf{v} + \boldsymbol{\sigma}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{v}) \right) + \int_{\partial\Omega_p} \frac{\rho\gamma}{\beta \Delta t} \mathbf{u} \cdot \mathbf{P} \cdot \mathbf{v} = \\ & \int_{\Omega} \frac{\rho}{\beta} \left(\frac{1}{\Delta t^2} \mathbf{u}_{\text{old}} \cdot \mathbf{v} + \frac{1}{\Delta t} \dot{\mathbf{u}}_{\text{old}} \cdot \mathbf{v} + \left(\frac{1}{2} - \beta \right) \ddot{\mathbf{u}}_{\text{old}} \cdot \mathbf{v} \right) + \\ & \int_{\partial\Omega_p} \left(\frac{\rho\gamma}{\beta \Delta t} \mathbf{u}_{\text{old}} \cdot \mathbf{P} \cdot \mathbf{v} + \left(\frac{\rho\gamma}{\beta} - \rho \right) \dot{\mathbf{u}}_{\text{old}} \cdot \mathbf{P} \cdot \mathbf{v} + \left(\frac{\rho\gamma \Delta t}{2\beta} - \rho \Delta t \right) \ddot{\mathbf{u}}_{\text{old}} \cdot \mathbf{P} \cdot \mathbf{v} \right). \end{aligned}$$

72 Here, (\mathbf{u}, \mathbf{v}) are the FEM trial and test functions, respectively, defined in FEM linear closed
73 space. $(\mathcal{U}, \mathcal{V})$ defined in $[H^1(\Omega)]^3$, for further details see PSD's soildynamics [documentation](#).

¹The *soildynamics* module builds upon the *elastodynamics* module by adding tools essential for earthquake modeling, such as paraxial boundary conditions, double-couple source mechanisms, point-cloud meshing-partitioning, etc.

74 **Execution Workflow:** PSD begins with automated code generation through the PSD_PreProcess
75 utility, which generates problem-specific FEM code based on user specifications.

76 PSD_PreProcess -problem soildynamics -dimension 3 -top2vol-meshing \
77 -timediscretization newmark_beta -postprocess uav

78 Typical soil properties and time-integration parameters are included:

```
79 real rho = 1800.0 , // Density
80     cs = 2300.0 , // S-wave velocity
81     cp = 4000.0 ; // P-wave velocity
82
83 real tmax = 20.0 , // Total time
84     t = 0.001 , // Initial time
85     dt = 0.001 ; // Time step
```

86 The simulation is executed using the parallel solver with the specified number of MPI-processes:

```
87 PSD_Solve -np 6144 Main.edp
```

88 Results such as those presented in Figure 1 can be obtained.

89 Demonstration

90 Figure 1 presents a regional-scale earthquake simulation of the Cadarache region in France (50
91 km × 50 km) performed with PSD (Badri et al., 2024), comprising over one billion degrees
92 of freedom distributed across 6144 MPI-domains on a 540-million-element mesh with 10 m
93 resolution.

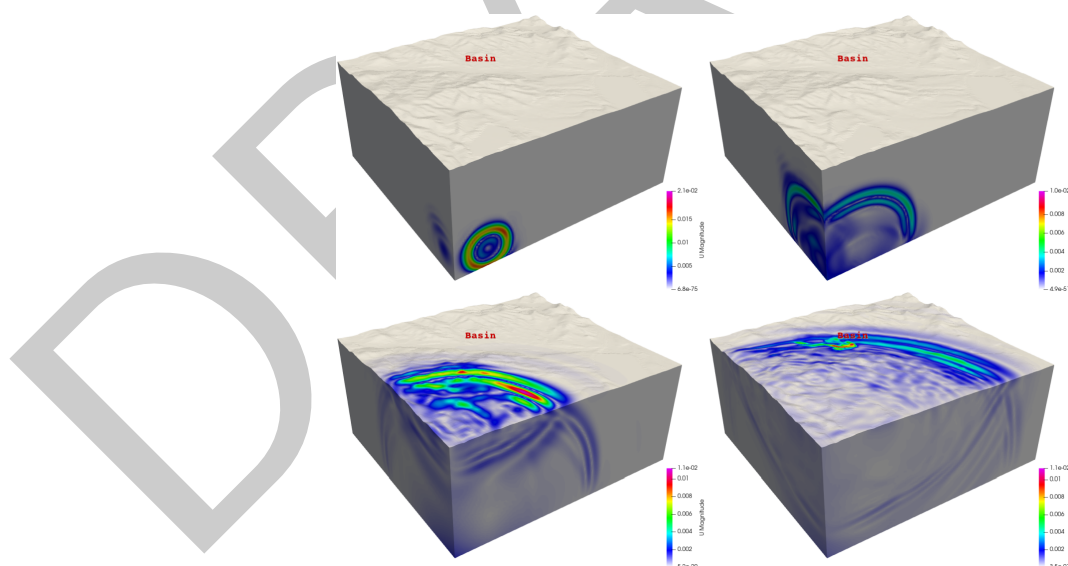


Figure 1: Earthquake simulation of the French Cadarache region showing displacement magnitude at four time steps.

94 Figure 2 demonstrates fracture mechanics capabilities through quasi-static brittle fracture
95 simulation in a perforated medium (Badri et al., 2021), involving more than 64 million degrees
96 of freedom across 1008 MPI-domains, illustrating detailed damage assessment capabilities.

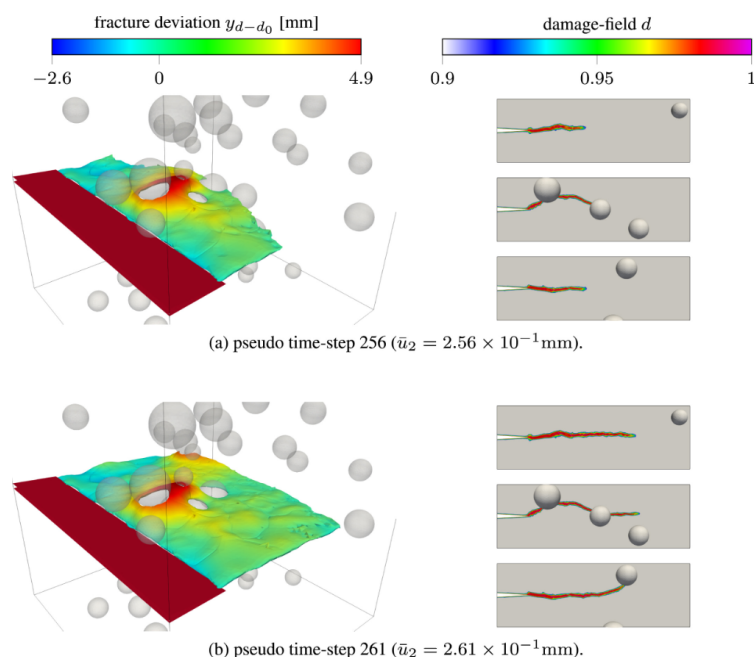


Figure 2: Crack propagation for a perforated medium.

These demonstrations represent significant computational achievements, with problem sizes approaching those required for seismic hazard and risk assessment. The Cadarache region simulation underscores PSD's applicability to real-world earthquake engineering, while the fracture mechanics case illustrates its capability for detailed damage analysis. Further applications, including eikonal non-local gradient damage models (Noigueira et al., 2023), (Nogueira et al., 2024), highlight PSD's versatility and its potential for comprehensive structural and fracture mechanics research.

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