Discontinuous Galerkin methods

Idea

- uses the **finite-element method** with a Galerkin approach for *piecewise* continuous functions and combines it with the concept of fluxes from **finite-volume methods**

- considers and discretizes the **weak form** of the equation(s):

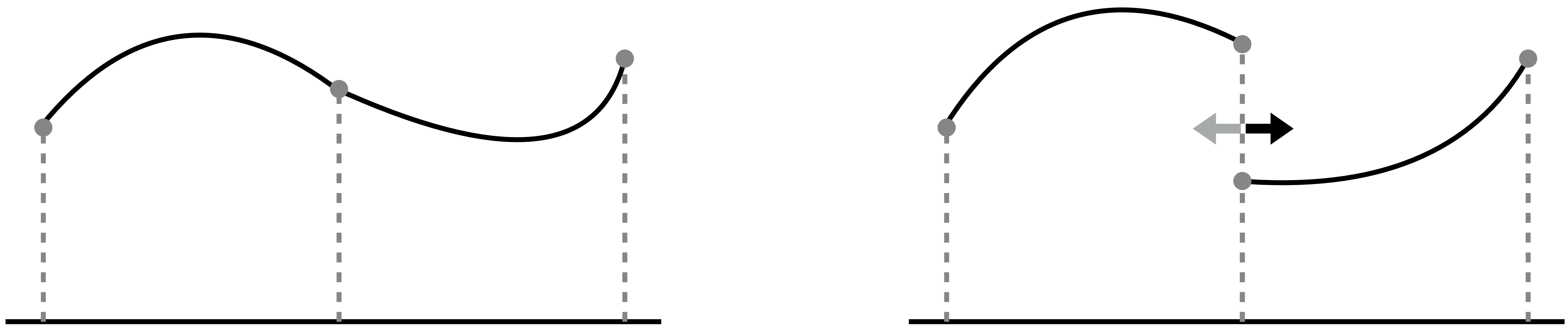
$$\partial_x^2 T + f = 0 \longrightarrow \int_0^L \mathsf{w}\, \partial_x^2 T \, \mathrm{d}x + \int_0^L \mathsf{w}\, f \, \mathrm{d}x = 0$$

- makes use of **Gauss' theorem** to compute the divergence of a quantity in term of its fluxes across element surfaces

$$\int_e \nabla \cdot (\mathsf{w}\, \nabla T) \, \mathrm{d}V = \int_{\partial e} \mathsf{w}\, \nabla T \cdot \hat{n} \, \mathrm{d}S$$

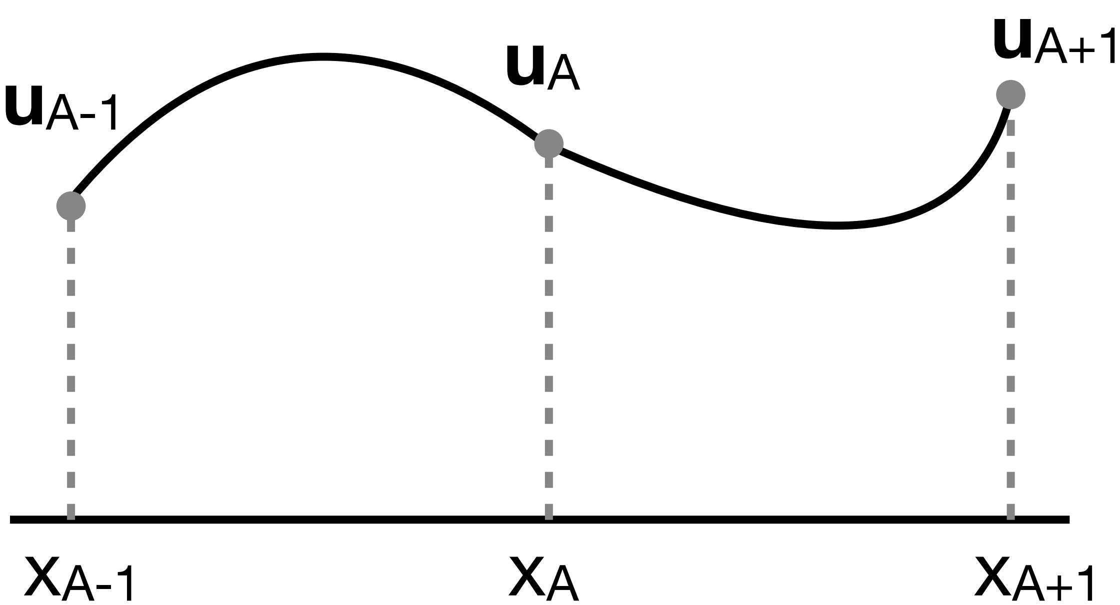
divergence ⟶ fluxes

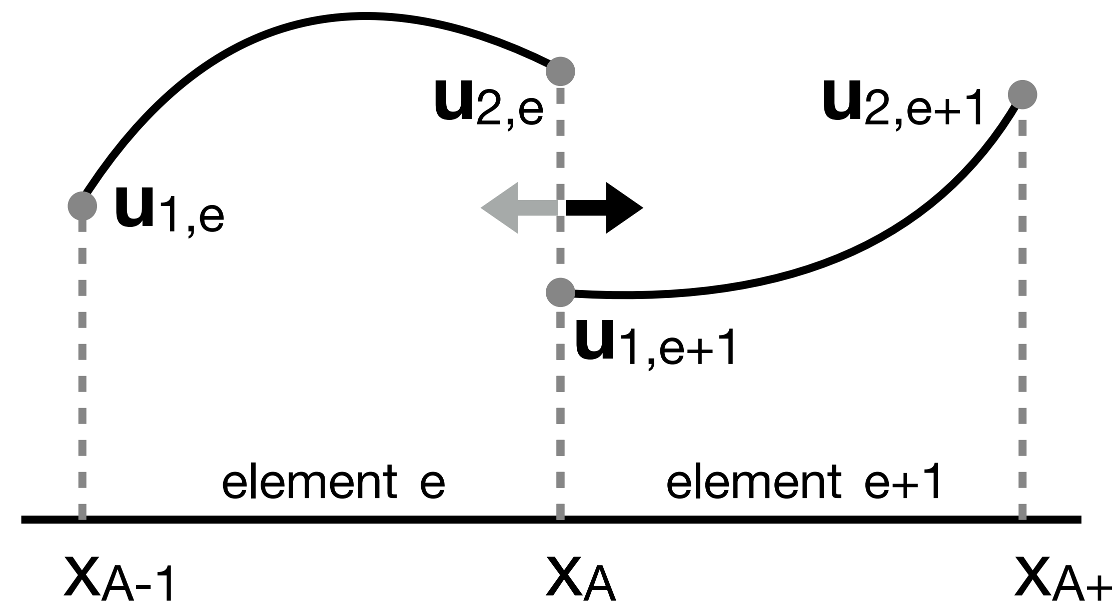
Idea



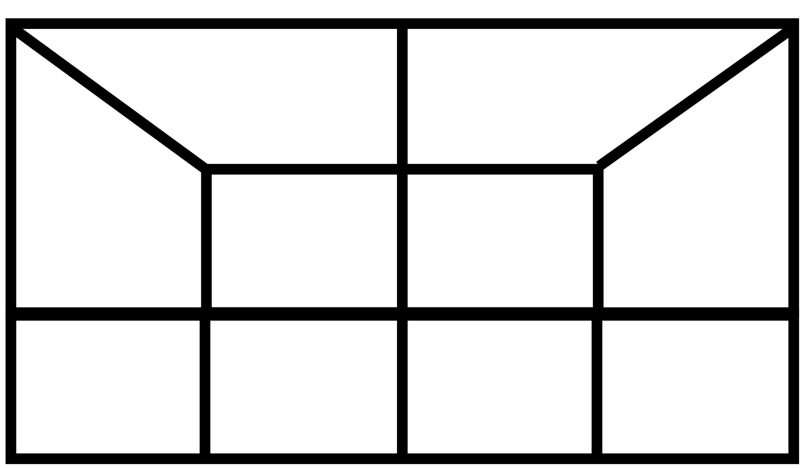
continuous → discontinuous

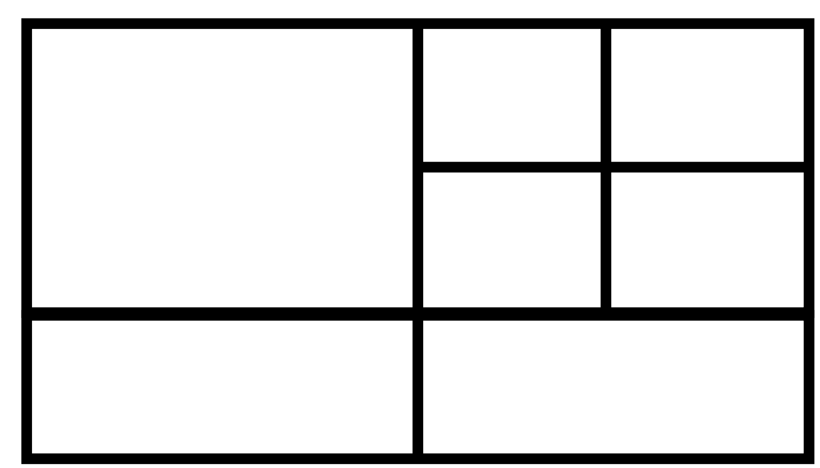
Idea





conforming → **non-conforming**





TRIANGULAR MESH METHODS FOR THE

NEUTRON TRANSPORT EQUATION

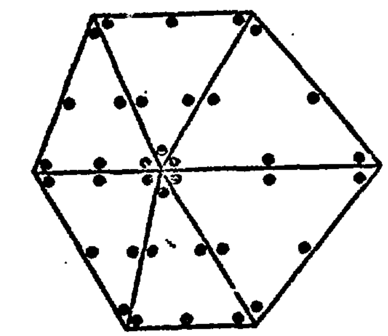


Fig. 4. A typical point arrangement for the discontinuous method. Boundary points are actually arbitrarily close to the boundary.

by

Wm. H. Reed and T. R. Hill

University of California,
Los Alamos Scientific Laboratory
Los Alamos, New Mexico 87544

ABSTRACT

The methods that are developed in this paper for differencing the discrete ordinates equations on a triangular x-y grid are based on piecewise polynomial representations of the angular flux. The first class of methods discussed here assumes continuity of the angular flux across all triangle interfaces. A second class of methods, which is shown to be superior to the first class, allows the angular flux to be discontinuous across triangle boundaries. Numerical results illustrating the accuracy and stability of these methods are presented, and numerical comparisons between the above two classes of methods are made. The effectiveness of a fine mesh rebalance acceleration technique is also discussed.

[Reed & Hill, 1971]

Geophys. J. Int. (2006) **166,** 855–877 doi: 10.1111/j.1365-246X.2006.03051.x

An arbitrary high-order discontinuous Galerkin method for elastic waves on unstructured meshes – I. The two-dimensional isotropic case with external source terms

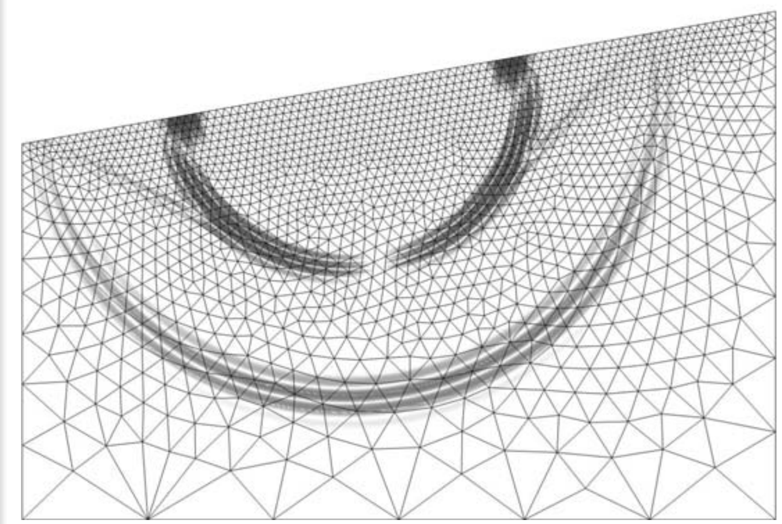
Martin Käser and Michael Dumbser

Department of Civil and Environmental Engineering, University of Trento, Trento, Italy. E-mail: martin.kaeser@ing.unitn.it

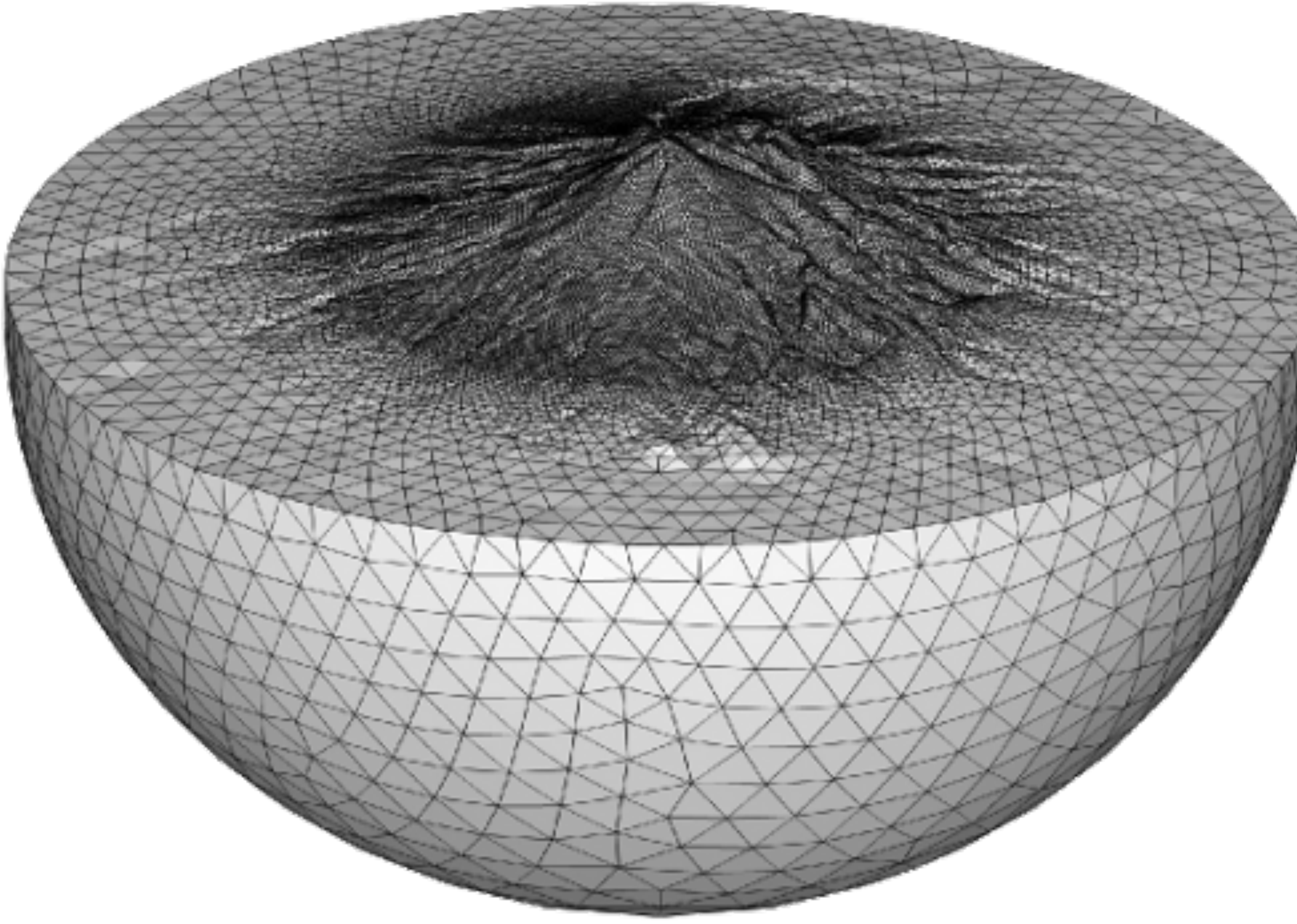
Accepted 2006 April 26. Received 2006 April 26; in original form 2005 April 7

SUMMARY

We present a new numerical approach to solve the elastic wave equation in heterogeneous media in the presence of externally given source terms with arbitrary high-order accuracy in space and time on unstructured triangular meshes. We combine a discontinuous Galerkin (DG) method with the ideas of the *ADER* time integration approach using *A*rbitrary high-order *DER*ivatives. The time integration is performed via the so-called Cauchy-Kovalewski procedure using repeatedly the governing partial differential equation itself. In contrast to classical finite element methods we allow for discontinuities of the piecewise polynomial approximation of the solution at element interfaces. This way, we can use the well-established theory of fluxes across element interfaces based on the solution of Riemann problems as developed in the finite volume framework. In particular, we replace time derivatives in the Taylor expansion of the time integration procedure by space derivatives to obtain a numerical scheme of the same high order in space *and* time using only one single explicit step to evolve the solution from one time level to another. The method is specially suited for linear hyperbolic systems such as the heterogeneous elastic wave equations and allows an efficient implementation. We consider continuous sources in space and time and point sources characterized by a Delta distribution in space and some continuous source time function. Hereby, the method is able to deal with point sources at *any* position in the computational domain that does not necessarily need to coincide with a mesh point. Interpolation is automatically performed by evaluation of test functions at the source locations. The convergence analysis demonstrates that very high accuracy is retained even on strongly irregular meshes and by increasing the order of the ADER–DG schemes computational time and storage space can be reduced remarkably. Applications of the proposed method to Lamb's Problem, a problem of strong material heterogeneities and to an example of global seismic wave propagation finally confirm its accuracy, robustness and high flexibility.

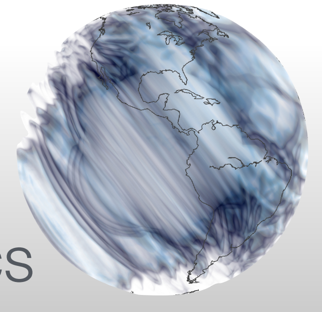


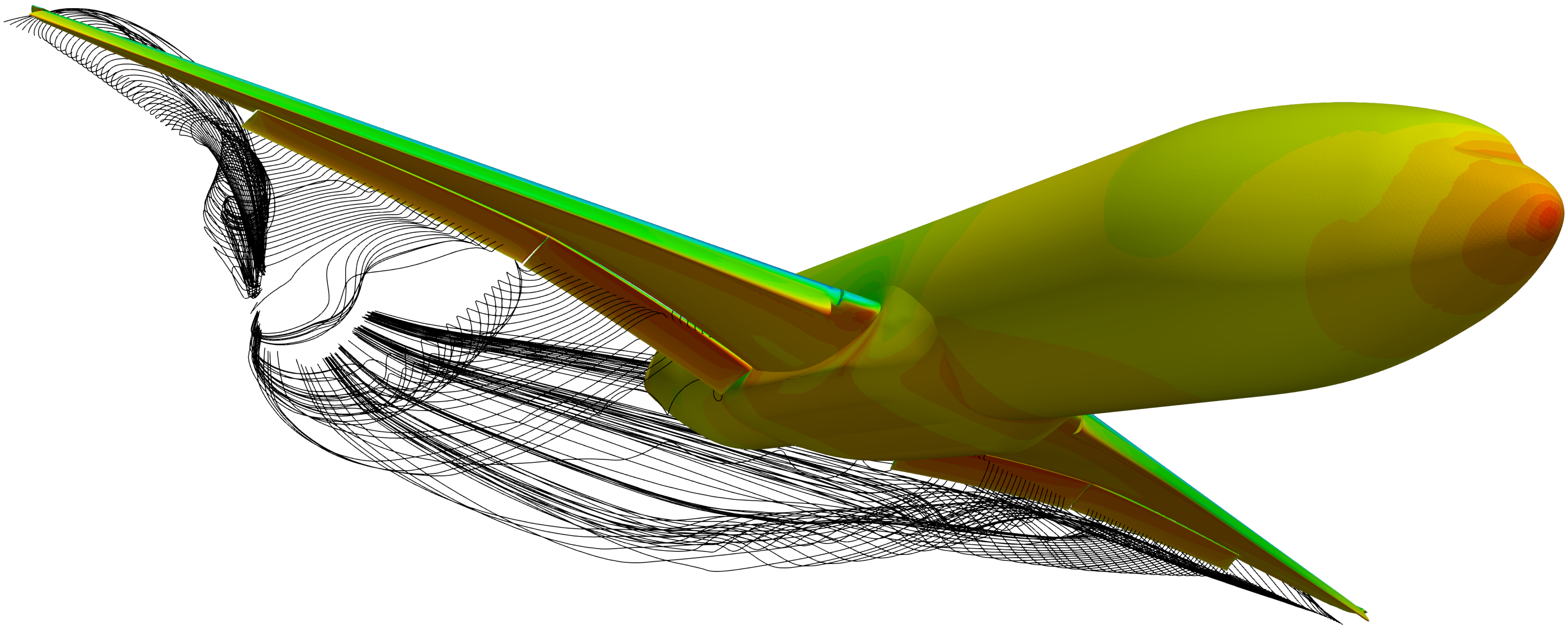
[Kaeser & Dumbser, 2006]



Seismology

SeisSol





Computational fluid dynamics
(DG for Euler & Navier-Stokes)

SU2

DG software

commercial

Comsol

..

open-source

SeisSol

exaDG

deal.II

FEniCSx

Nektar++

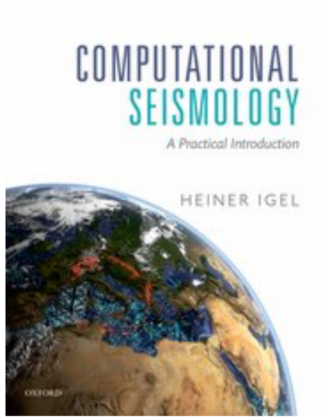
FreeFEM

MFEM

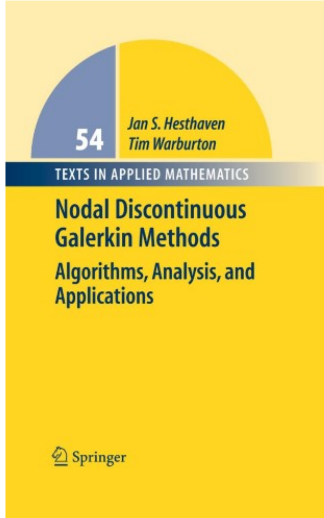
..

DG literature

books



H. Igel
Computational Seismology
Oxford Press University, 2016.



J. S. Hesthaven, T. Warburton
Nodal Discontinuous Galerkin Methods,
Springer, 2008.

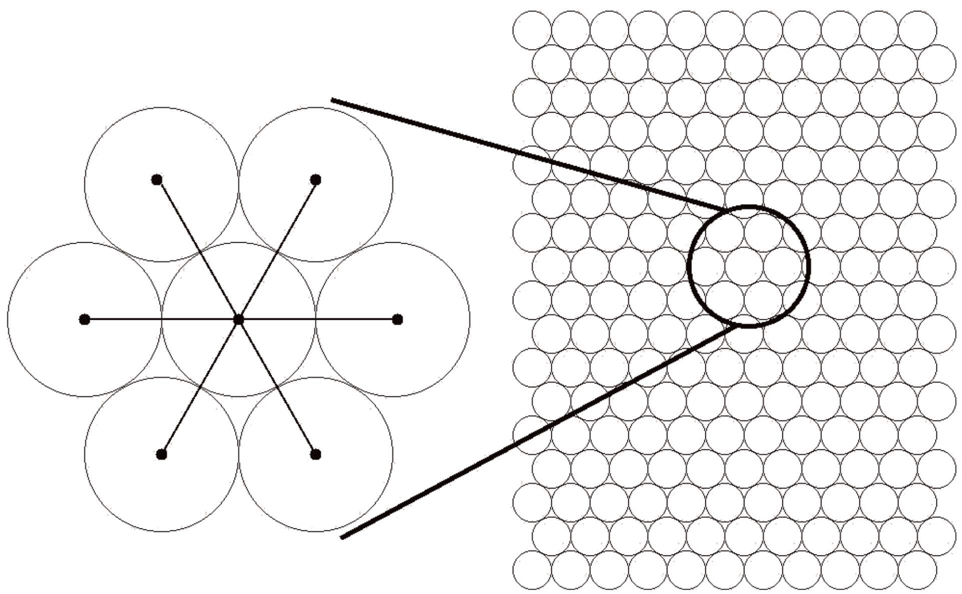
online tutorials

https://youtu.be/E9_kyXjtRHc - Aidan Wimshurst, Fluid mechanics 101

Lattice-Boltzmann methods
Elastic lattice methods
Discrete particle methods

Idea

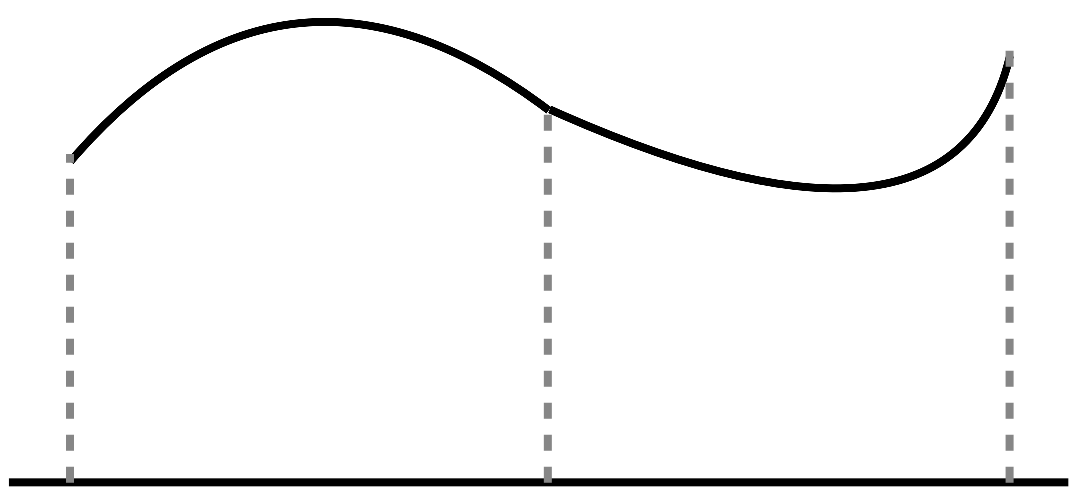
- uses **discrete particles** with a given mass, position & velocity to simulate a fluid/elastic medium

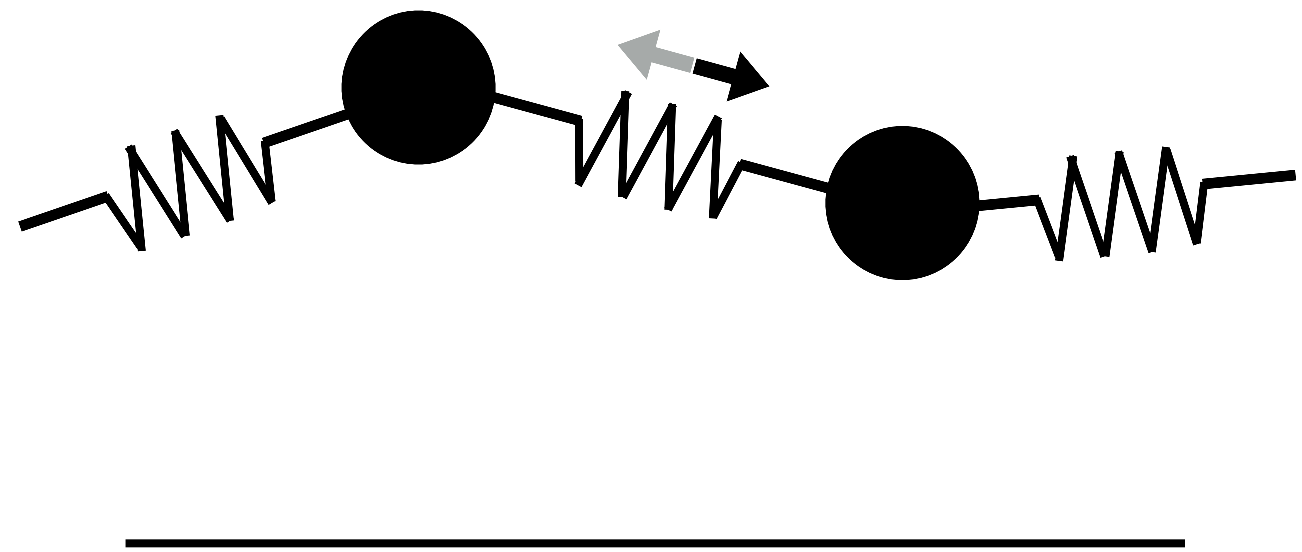


- solving this system involves a
  collision (particle-particle interaction) and a
  streaming (positional update) step

- for wave propagation modeling, the particle interaction is based on **Hooke's law** to compute the forces acting on each particle, while the positional update is given by **Newtonian dynamics**

Idea





continuous → **particles**

Geophys. J. Int. (2000) **141,** 595–604

Numerical simulation of seismic waves using a discrete particle scheme

Aoife Toomey and Christopher J. Bean
Department of Geology, University College Dublin, Belfield, Dublin 4, Ireland

Accepted 1999 December 3. Received 1999 December 3; in original form 1999 February 1

SUMMARY

A particle-based model for the simulation of wave propagation is presented. The model is based on solid-state physics principles and considers a piece of rock to be a Hookean material composed of discrete particles representing fundamental intact rock units. These particles interact at their contact points and experience reversible elastic forces proportional to their displacement from equilibrium. Particles are followed through space by numerically solving their equations of motion. We demonstrate that a numerical implementation of this scheme is capable of modelling the propagation of elastic waves through heterogeneous isotropic media. The results obtained are compared with a high-order finite difference solution to the wave equation. The method is found to be accurate, and thus offers an alternative to traditional continuum-based wave simulators.

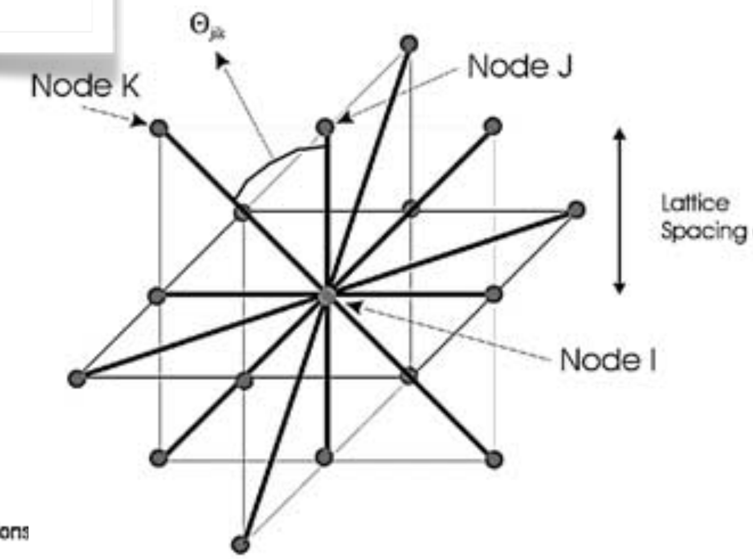
[Toomey & Bean, 2000]

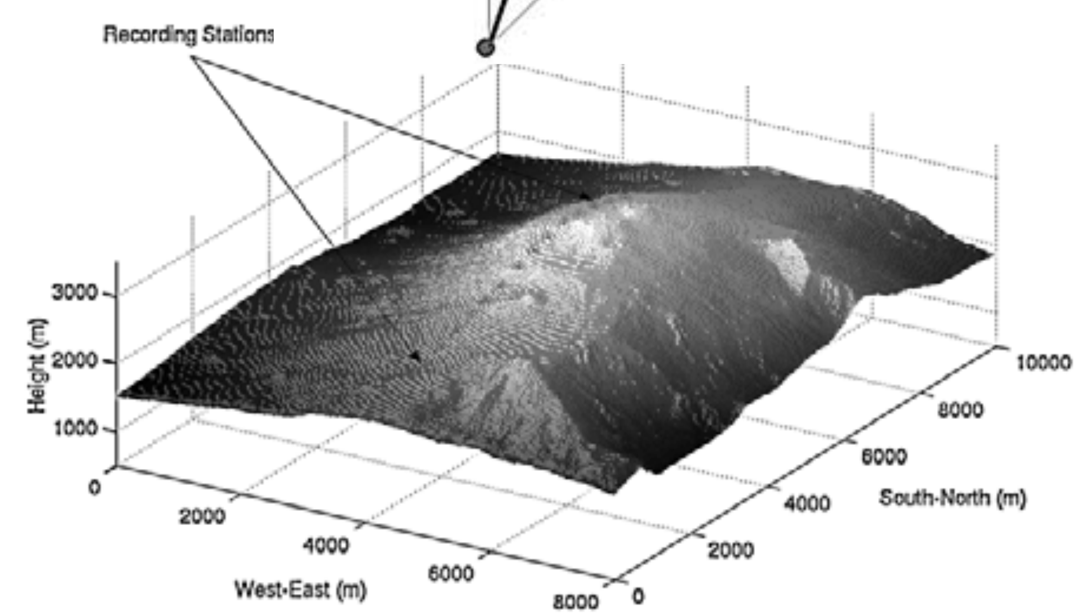
GEOPHYSICAL RESEARCH LETTERS, VOL. 31, L14608, doi:10.1029/2004GL020069, 2004

A 3D discrete numerical elastic lattice method for seismic wave propagation in heterogeneous media with topography

Gareth S. O'Brien and Christopher J. Bean

[1] A three-dimensional elastic lattice method for the simulation of seismic waves is presented. The model consists of particles arranged on a cubic lattice which interact through a central force term and a bond-bending force. Particle disturbances are followed through space by numerically solving their equations of motion. A vacuum free-surface boundary condition is implicit in the method. We demonstrate that a numerical implementation of the method is capable of modelling seismic wave propagation with complex topography. This is achieved by comparing the scheme against a finite-difference solution to the elastodynamic wave equation. The results indicate that the scheme offers an alternative 3D method for modelling wave propagation in the presence of strong topography and subsurface heterogeneity. We apply the method to seismic wave propagation on Mount Etna to illustrate its applicability in modelling a physical system. *INDEX TERMS:* 3210





[O'Brien & Bean, 2004]

Geophys. J. Int. (2007) **171,** 857–864 doi: 10.1111/j.1365-246X.2007.03579.x

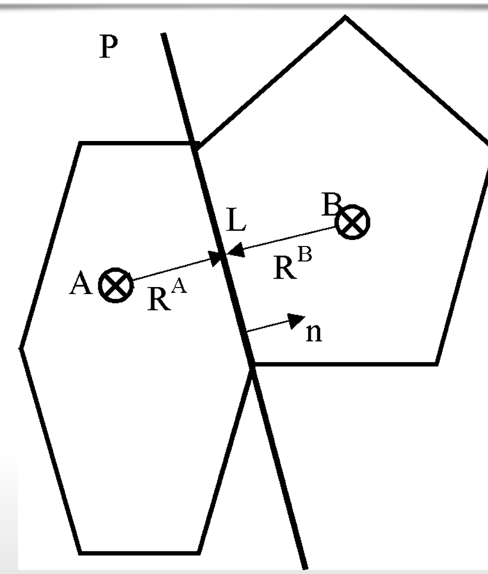
Lamb's problem with the lattice model Mka3D

C. Mariotti
C.E.A./D.A.M. Laboratoire de Détection et de Géophysique, 91680 *Bruyères le Châtel, France. E-mail: christian.mariotti@cea.fr*

Accepted 2007 August 6. Received 2007 May 16; in original form 2007 January 26

SUMMARY
A lattice model has been developed in 2-D in the code Mka3D. Our aim is to evaluate the capability of this method to be used for seismic wave propagation. After a description of the particle interaction, the simulation of the seismic Lamb's test in 2-D is compared with the analytical solution for several values of elastic properties. Finally, wave propagation in a sedimentary basin is simulated both with Mka3D and a Spectral Element Method (SEM), and both solutions are compared.

[Mariotti, 2007]



Computational Geophysics

Bulletin of the Seismological Society of America, Vol. 102, No. 3, pp. 1224–1234, June 2012, doi: 10.1785/012011019

A Lattice Boltzmann Method for Elastic Wave Propagation in a Poisson Solid

by G. S. O'Brien,* T. Nissen-Meyer, and C. J. Bean

Abstract The lattice Boltzmann (LB) method is a numerical method that has its origins in discrete mechanics. The method is based on propagating discrete density distributions across a fixed lattice and implementing conservation laws between the density distributions at lattice intersections. The method has been successfully applied to a wide variety of problems in fluid dynamics but has yet to be applied to elastic wave propagation. In this article we outline a new 2D and 3D LB solution to the elastic wave equation in a Poisson solid using a regular lattice, in 2D a square geometry and in 3D a cubic geometry. We outline the theory behind the method and derive the elastic wave equation from a Chapman–Enskog expansion about the Knudsen number. The scheme is shown to give rise to the elastic wave equation with a fixed Poisson ratio of 0.25 with a Knudsen number truncation error of order two. We have performed a von Neumann plane-wave analysis and found that the numerical dispersion is comparable to other discrete methods for modelling wave propagation. We have compared the numerical method to two problems, a 3D infinite homogeneous medium and a 2D heterogeneous block model. In both cases, we found the solutions agreed, thus showing that the LB method can be used to model elastic wave propagation. The scheme offers the potential to model the interaction of several continuum equations within one solver as the continuum equation is solely dependent on the equilibrium distribution.

[O'Brien et al., 2012]

Modelling viscoacoustic wave propagation with the lattice Boltzmann method

Muming Xia[1], Shucheng Wang[1], Hui Zhou[1], Xiaowen Shan[1,2,3], Hanming Chen[1], Qingqing Li[1] & Qingchen Zhang[1]

In this paper, the lattice Boltzmann method (LBM) is employed to simulate wave propagation in viscous media. LBM is a kind of microscopic method for modelling waves through tracking the evolution states of a large number of discrete particles. By choosing different relaxation times in LBM experiments and using spectrum ratio method, we can reveal the relationship between the quality factor Q and the parameter τ in LBM. A two-dimensional (2D) homogeneous model and a two-layered model are tested in the numerical experiments, and the LBM results are compared against the reference solution of the viscoacoustic equations based on the Kelvin-Voigt model calculated by finite difference method (FDM). The wavefields and amplitude spectra obtained by LBM coincide with those by FDM, which demonstrates the capability of the LBM with one relaxation time. The new scheme is relatively simple and efficient to implement compared with the traditional lattice methods. In addition, through a mass of experiments, we find that the relaxation time of LBM has a quantitative relationship with Q. Such a novel scheme offers an alternative forward modelling kernel for seismic inversion and a new model to describe the underground media.

[Xie et al., 2017]

LBM software

open-source

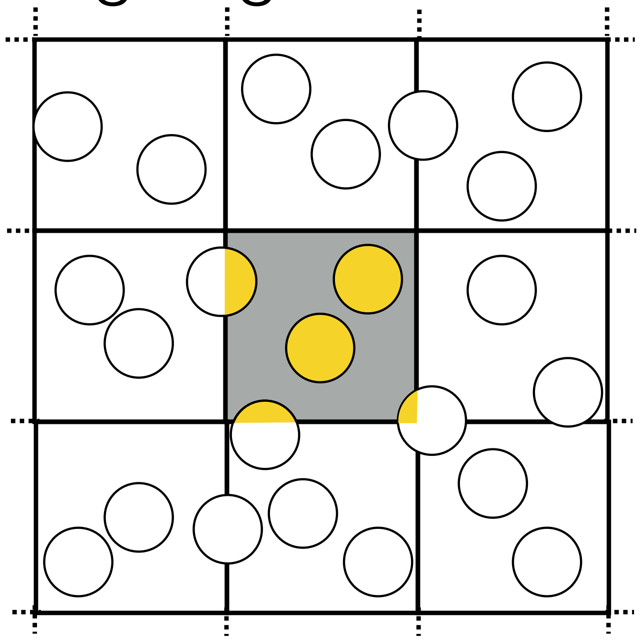
Mka3D - discrete element method

..

Particle-in-cell methods

Idea

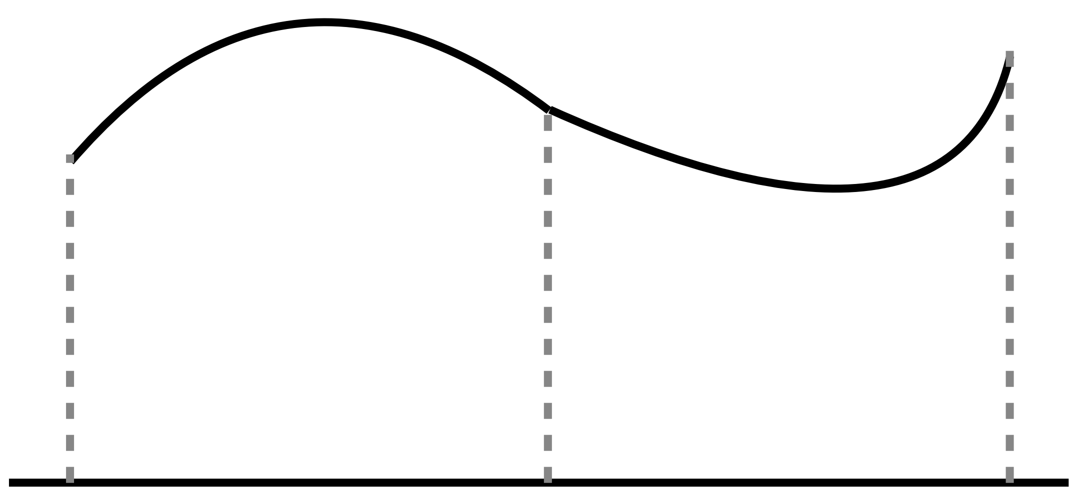
- combines solving (velocity) **fields on Eulerian** grids with **discrete tracers** in a Lagrangian framework

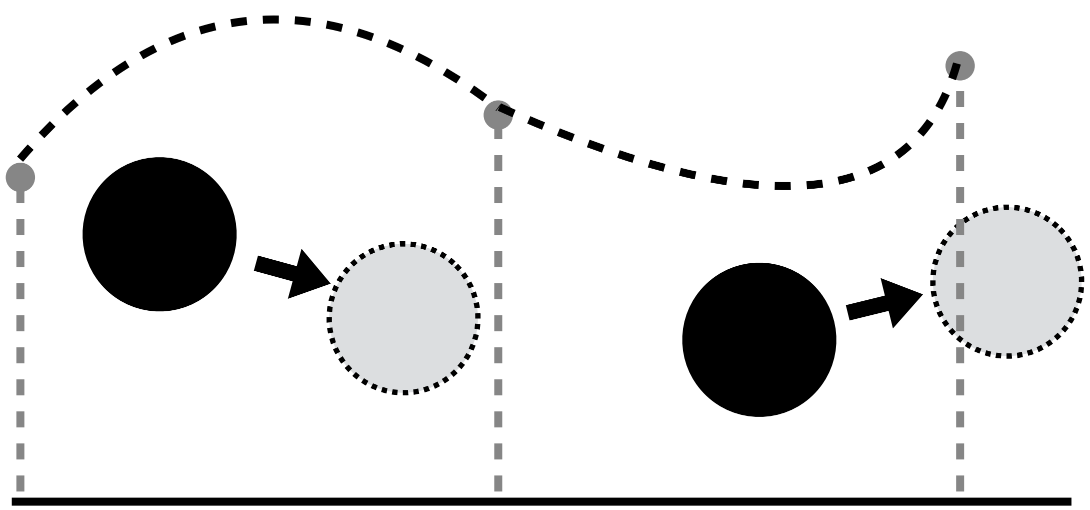


- for geodynamics, motivated by advection problems and how **distinct particles** would be transported by an external flow field

- solves the field equations, e.g., by a finite-differences/finite-element/.. method on a fixed grid, and **interpolates between fields & particles situated anywhere** in the domain (by particle-mesh & mesh-particle interactions in corresponding grid cells)

Idea





continuous $\longrightarrow$ **field & tracers**

THE PARTICLE-IN-CELL METHOD

FOR NUMERICAL SOLUTION OF PROBLEMS IN FLUID DYNAMICS

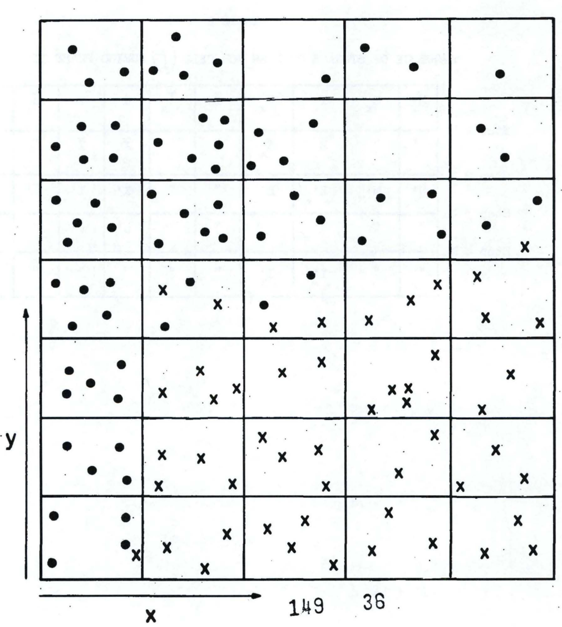
Francis H. Harlow

LADC-5288

The University of California, Los Alamos Scientific Laboratory
Los Alamos, New Mexico

ABSTRACT

The Particle-in-Cell method is a procedure to be used on high-speed computer for studies of the dynamics of compressible fluids undergoing large distortions. The technique is described in detail for calculation of the dynamics of two fluids confined to move in a two-dimensional rectangular box, and techniques are discussed for the extension to numerous other types of problems. Discussion is also given of many properties, limitations and uses of the method, which have been learned through the application to a wide variety of problems.



[Harlow, 1962]

Geochemistry Geophysics Geosystems G3
AN ELECTRONIC JOURNAL OF THE EARTH SCIENCES
Published by AGU and the Geochemical Society

Technical Brief
Volume 4, Number 4
22 April 2003
8302, doi:10.1029/2001GC000214
ISSN: 1525-2027

Testing the tracer ratio method for modeling active compositional fields in mantle convection simulations

Paul J. Tackley
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Scott D. King
Department of Earth and Atmospheric Sciences, Purdue University, 550 Stadium Mall Drive, West Lafayette, Indiana 47907, USA (sking@purdue.edu)

[Tackley & King, 2003]

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Available online at www.sciencedirect.com
SCIENCE DIRECT®
Physics of the Earth and Planetary Interiors 140 (2003) 293–318
PHYSICS OF THE EARTH AND PLANETARY INTERIORS
www.elsevier.com/locate/pepi

Characteristics-based marker-in-cell method with conservative finite-differences schemes for modeling geological flows with strongly variable transport properties

Taras V. Gerya[a,b,*], David A. Yuen[c]

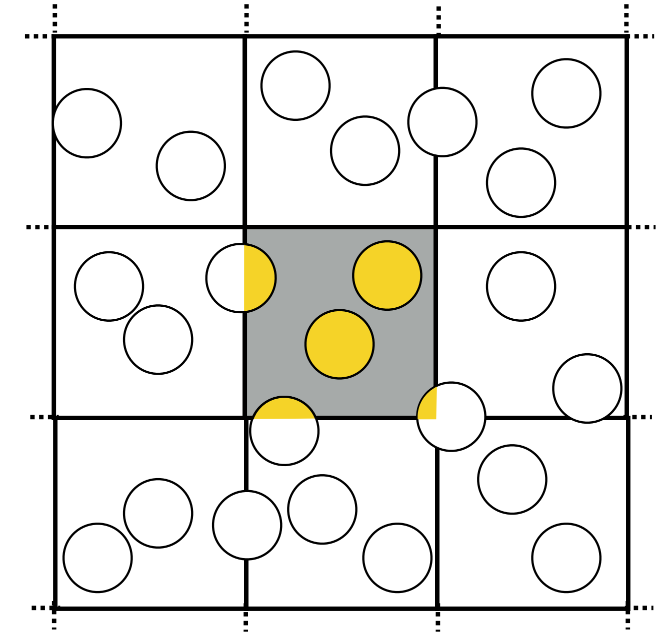
[Gerya & Yuen, 2003]

Geophys. J. Int. (2018) 214, 1744–1773
doi: 10.1093/gji/ggy231
Advance Access publication 2018 June 12
GJI Geodynamics and tectonics

A deformable particle-in-cell method for advective transport in geodynamic modelling

Henri Samuel[1,2]

[Samuel, 2018]



Geochemistry, Geophysics, Geosystems

TECHNICAL REPORTS: METHODS

10.1029/2018GC007508

Flexible and Scalable Particle-in-Cell Methods With Adaptive Mesh Refinement for Geodynamic Computations

Rene Gassmöller[1], Harsha Lokavarapu[1], Eric Heien[2], Elbridge Gerry Puckett[3], and Wolfgang Bangerth[4]

[Gassmoeller et al., 2018]

PiC software

open-source

mantle convection:

ASPECT

Ellipsis3D

short-term crustal dynamics:

PyLith

..

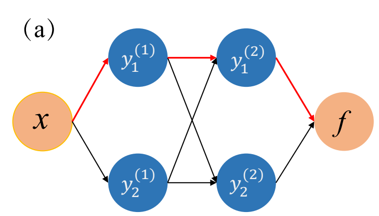
Physics-Informed Neural Networks

Idea

- uses a **deep neural network** as a function approximator

- training adds the partial differential equations of the **physics as loss terms**, making it a constraint optimization problem, together with supervised learning on a (sparse) sampling of the solution field (collocation points)

- takes advantage of **automatic differentiation** to compute derivatives in the loss terms, relying on differentiable neural network activation functions (such as hyperbolic tangent, sine, ELU, Swish, ..)

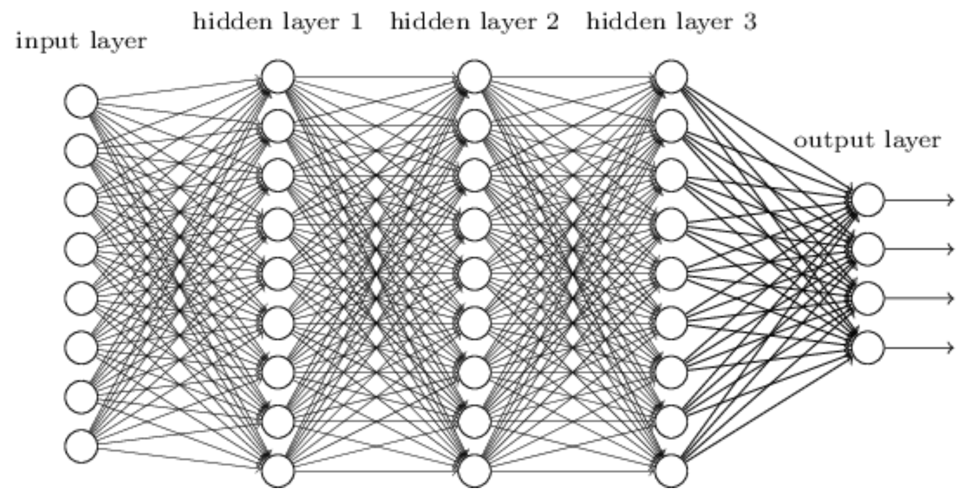


(b)

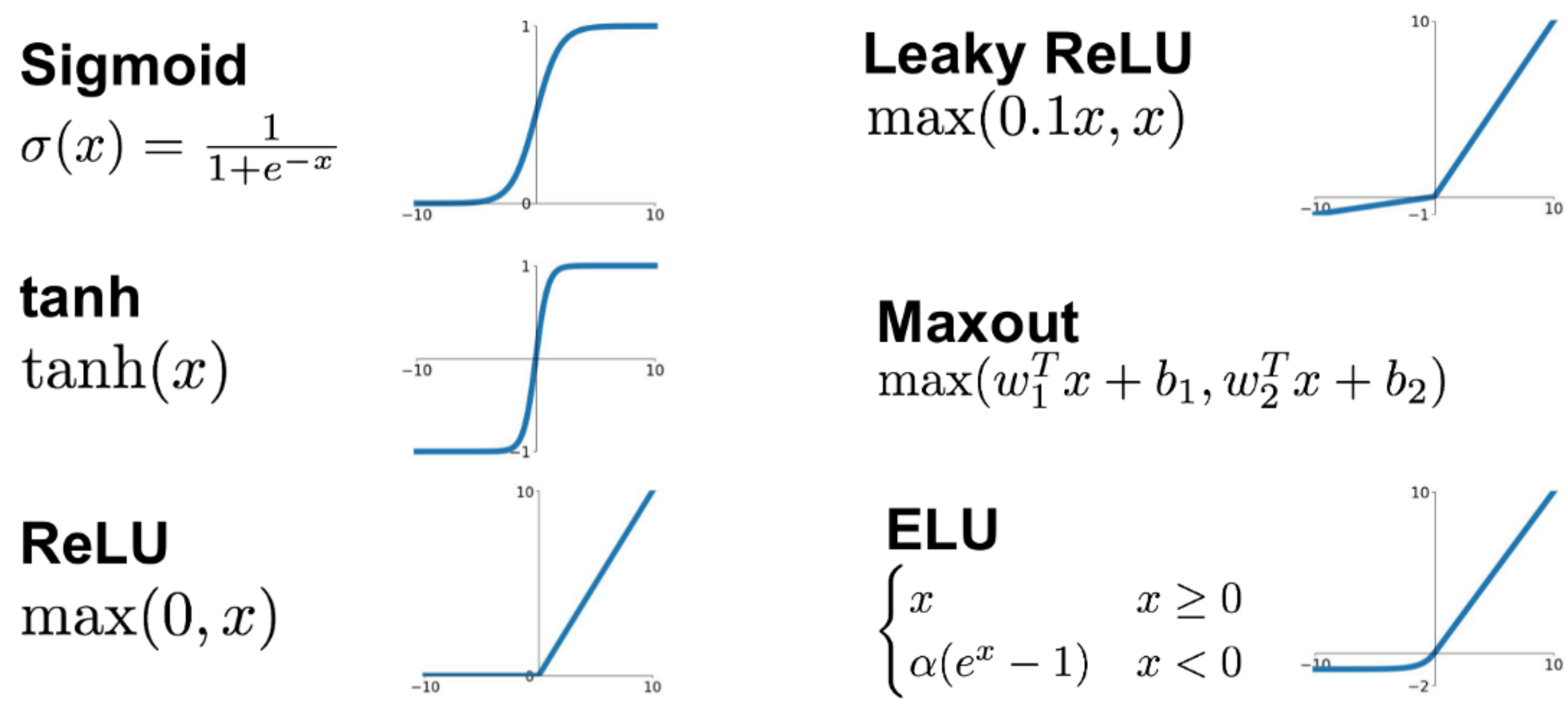
$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial y_1^{(2)}} \frac{\partial y_1^{(2)}}{\partial y_1^{(1)}} \frac{\partial y_1^{(1)}}{\partial x} + \frac{\partial f}{\partial y_1^{(2)}} \frac{\partial y_1^{(2)}}{\partial y_2^{(1)}} \frac{\partial y_2^{(1)}}{\partial x} + \frac{\partial f}{\partial y_2^{(2)}} \frac{\partial y_2^{(2)}}{\partial y_1^{(1)}} \frac{\partial y_1^{(1)}}{\partial x} + \frac{\partial f}{\partial y_2^{(2)}} \frac{\partial y_2^{(2)}}{\partial y_1^{(1)}} \frac{\partial y_1^{(1)}}{\partial x}$$

Idea

- fully-connected neural network for deep learning



- activation functions



Idea

- neural networks usually exhibit a “spectral bias”, i.e., a preference for low-frequency solutions
  -> transform input by high-frequency functions:
  Fourier networks
  -> using periodic activation functions (sine):
  SiReNs

- PINNs can handle both strong- and weak-form descriptions of the partial differential equations

$$\begin{cases} -\Delta u = f & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases} \longrightarrow \begin{aligned} \int_\Omega \nabla u \cdot \nabla v dx &= \int_\Omega f v dx \\ u &= 0 \quad \text{on } \partial\Omega \end{aligned}$$

Idea

continuous → **approximated by NN**

Journal of Computational Physics 378 (2019) 686–707

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations

M. Raissi [a], P. Perdikaris [b,*], G.E. Karniadakis [a]

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A R T I C L E   I N F O

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Available online 3 November 2018

Keywords:
Data-driven scientific computing
Machine learning
Predictive modeling
Runge–Kutta methods
Nonlinear dynamics

A B S T R A C T

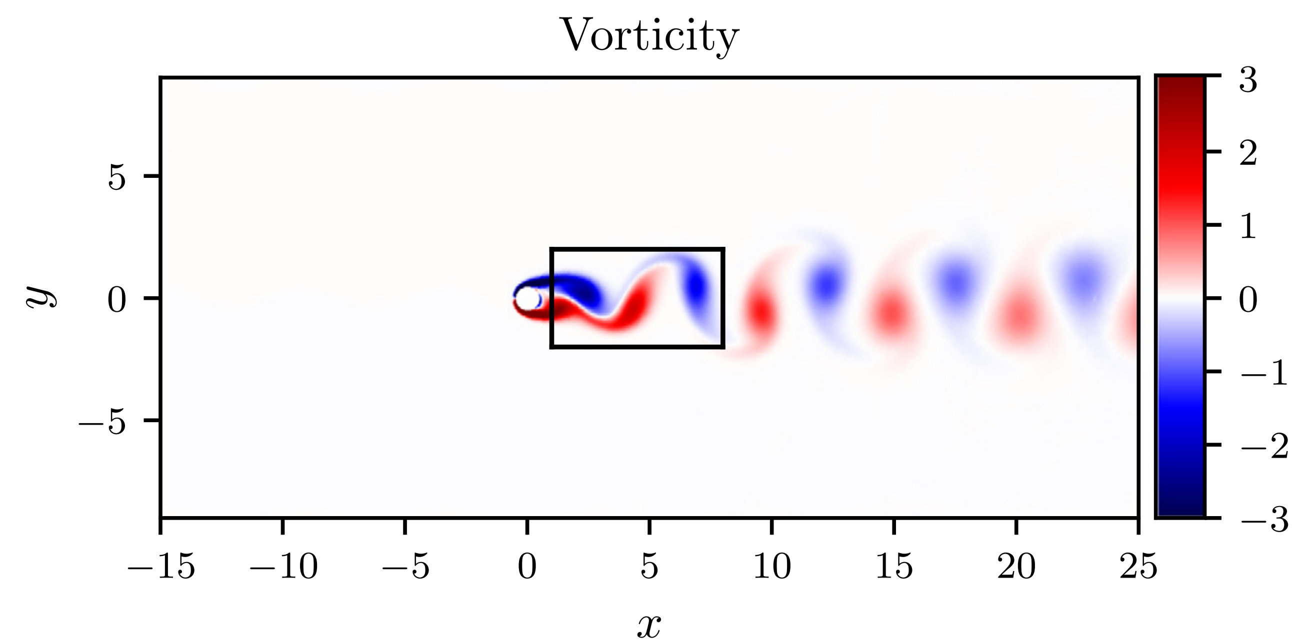
We introduce *physics-informed neural networks* – neural networks that are trained to solve supervised learning tasks while respecting any given laws of physics described by general nonlinear partial differential equations. In this work, we present our developments in the context of solving two main classes of problems: data-driven solution and data-driven discovery of partial differential equations. Depending on the nature and arrangement of the available data, we devise two distinct types of algorithms, namely continuous time and discrete time models. The first type of models forms a new family of *data-efficient* spatio-temporal function approximators, while the latter type allows the use of arbitrarily accurate implicit Runge–Kutta time stepping schemes with unlimited number of stages. The effectiveness of the proposed framework is demonstrated through a collection of classical problems in fluids, quantum mechanics, reaction–diffusion systems, and the propagation of nonlinear shallow-water waves.

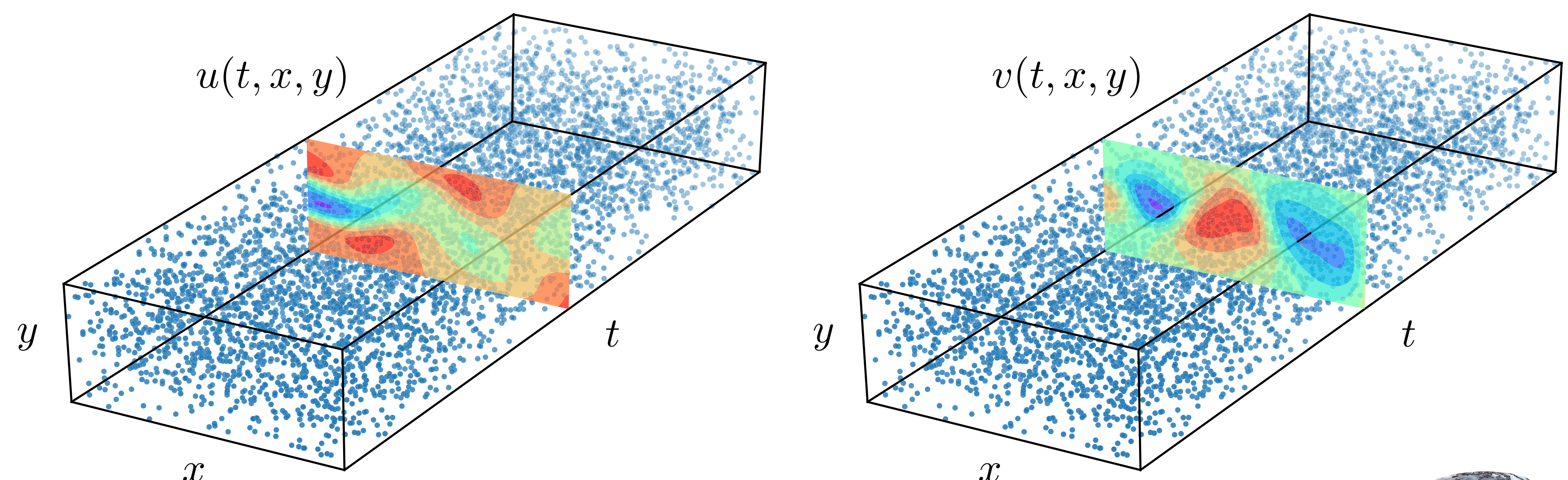
[Raissi et al., 2019]

Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations

M. Raissi [a], P. Perdikaris [b,*], G.E. Karniadakis [a]

Navier-Stokes equation example





[Raissi et al., 2019]

Applications: wave equation

Implicit Neural Representations with Periodic Activation Functions

Vincent Sitzmann* sitzmann@cs.stanford.edu
Julien N. P. Martel* jnmartel@stanford.edu
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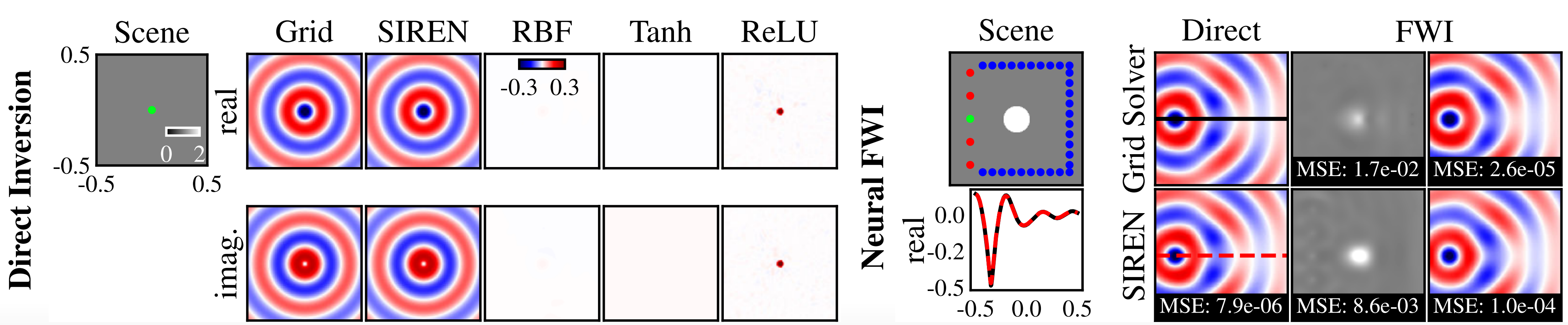
Gordon Wetzstein gordon.wetzstein@stanford.edu

Stanford University
vsitzmann.github.io/siren/

[Sitzmann et al., 2020] https://github.com/vsitzmann/siren



Applications: wave equation

Physics-informed Neural Networks (PINNs) for Wave Propagation and Full Waveform Inversions

Majid Rasht-Behesht[1], Christian Huber[1], Khemraj Shukla[2] and George Em Karniadakis[3]

[Rasht-Behesht et al., 2021] https://doi.org/10.26300/x3wd-4k56

Physics informed deep learning for computational elastodynamics without labeled data

Chengping Rao[a], Hao Sun[b,c], Yang Liu[a,*]

[Rao et al., 2021] https://github.com/Raocp/PINN-elastodynamics

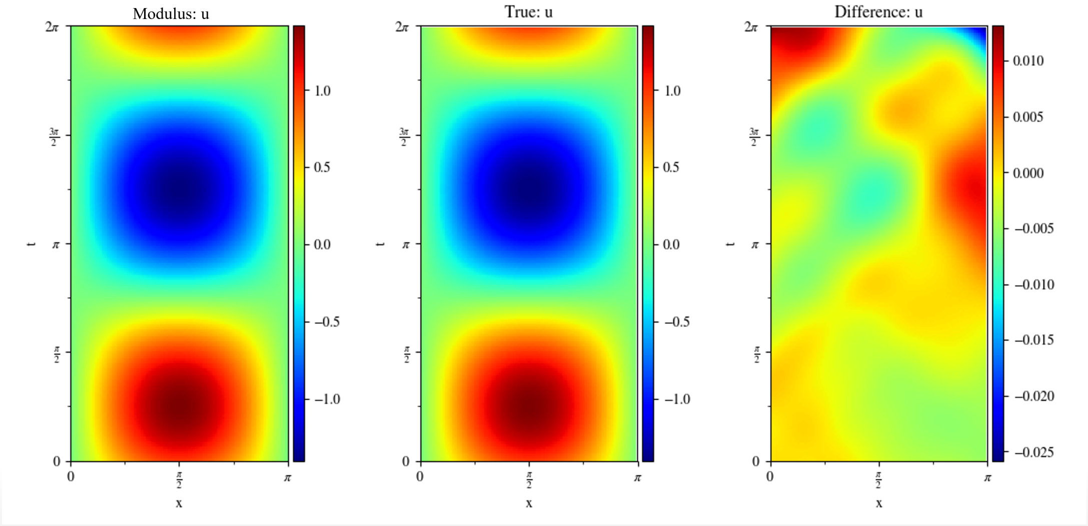
Applications: wave equation

Nvidia modulus example:

$$
\begin{aligned}
u_{tt} &= c^2 u_{xx} \\
u(0,t) &= 0, \\
u(\pi,t) &= 0, \\
u(x,0) &= \sin(x), \\
u_t(x,0) &= \sin(x).
\end{aligned}
$$

steps:

1. describe equation (using simpy)
2. setup geometry
3. define a range of sampling/collocation points (in space & time)
4. generate validation data (using analytical/numerical solvers)
5. create neural net (fully-connected, Fourier net, SiReN, ..)
   & a loss term weighting scheme
6. train, solve, predict…



PINN software

open-source

Nvidia Modulus (examples provided)

pyTorch

tensorFlow

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