PyAspect:
Workflow and automation tools for SPECFEM3D

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BACKGROUND

Solving for 3D inversions of either source or subsurface properties is computationally expensive and requires complex workflows. Furthermore, limited software packages are available for high-fidelity 3D inversions of regions with complex geological structure. One such region with complex geological subsurface structure, is the Groningen filed. To date, we are aware of only one open-source software package that can be used for calculating sufficient 3D inversion of the Groningen field. This is the SPECFEM3D-Cartesian package (SPEC). Unfortunately, full workflows for 3D inversion are not integrated into SPEC, and the codes for different steps of the workflow consist of a patchwork of individual applications or packages. Therefore, it is difficult to track and document, in a reproducible manner, any parameter changes used, or any intermediate data produced during specific workflow steps. In our attempt to compute 3D inversions for the Groningen field, we developed codes to improve the reproducibility and automation of inversion workflows with respect to SPEC. It should be noted that several years ago a Python package, SeisFlows (Modrak, et al., 2016), was developed which attempted to consolidate inversion workflows for SPEC, but that package appears to have become antiquated with respect to the SPEC codes and Python.

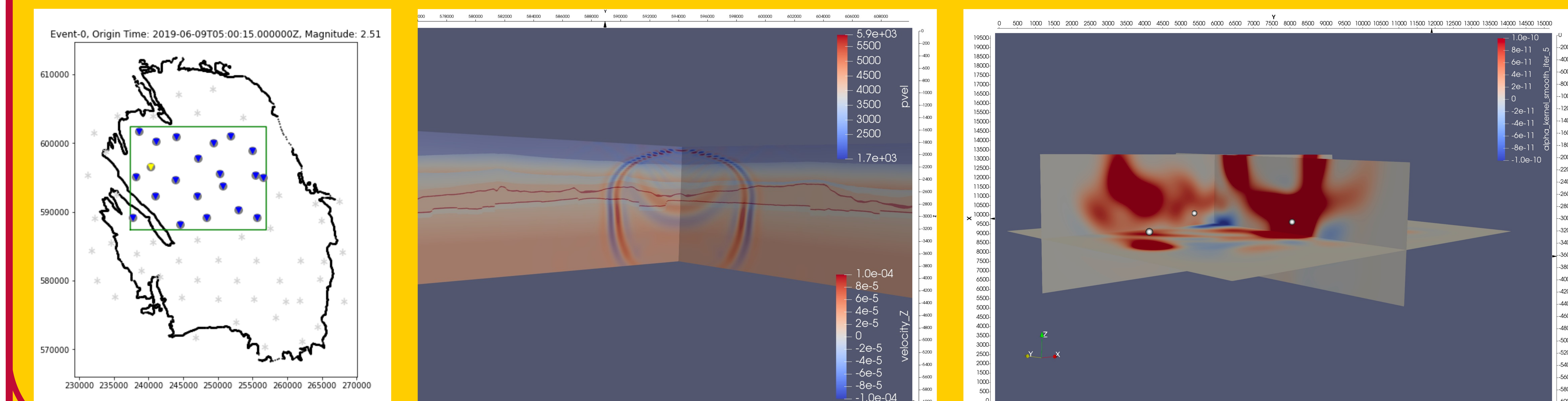
MEHTODS

We developed the PyAspect package to be as consistent as possible with the reproducible environment described by Beg, et al., 2019.

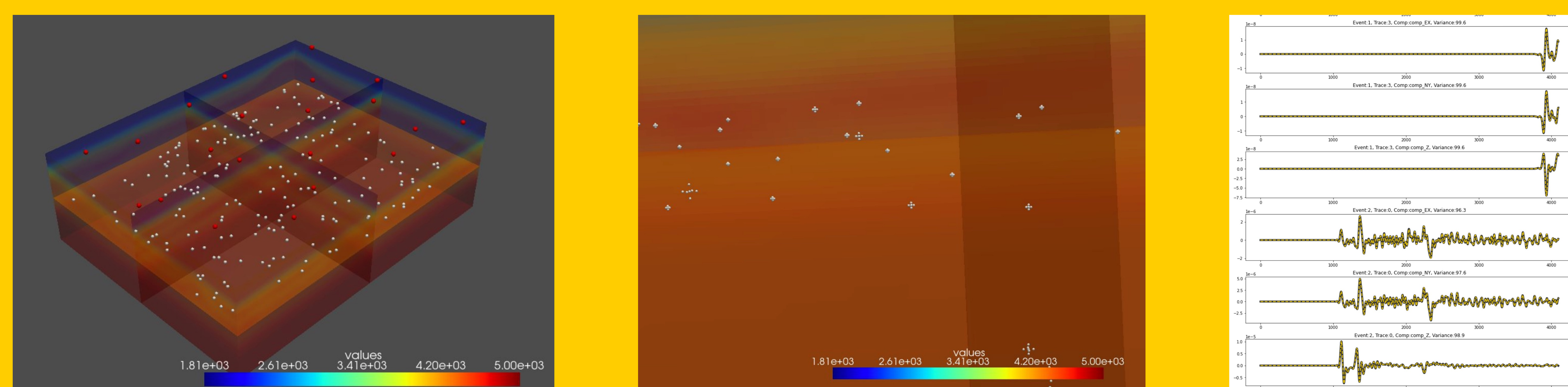
- **Open-source** via github.com
- **Python** is primary code base
- **Pythonic** functions and data structures
- **Jupyter Notebooks** for data analysis and setting up HPC SPEC executions environment
- **Infinite headers**: dictionaries-to-pandas and vis versa.
- **Data-science** friendly
- **Flexible HPC environments**: Shell-scripts for SPEC inversion steps and iterations

Reproducible and Re-usable: Automated workflow tools for 3D seismic inversion

Forward modeling and inversion



Moment-tensors and reciprocity



Online version and more info

Why this poster layout?

RESULTS

- Convert gridded models to meshed SPEC models
- Interactively view 3D models in Jupyter Notebooks
- Convert source and receiver (station) headers and data to conventional SPEC data files and vis versa
- Create SPEC project for specific HPC environments including for:
  - Forward modeling
  - Inversion
  - Reciprocity
- Modular shell-scripts for SPEC inversion steps and iterations
- Reciprocal moment-tensors

REFERENCES

- M. Beg et al., "Using Jupyter for Reproducible Scientific Workflows," in Computing in Science & Engineering, vol. 23, no. 2, pp. 36-46, 1 March-April 2021, doi: 10.1109/MCSE.2021.3052101.
- Ryan T. Modrak, Dmitry Borisov, Matthieu Lefebvre, Jeroen Tromp, SeisFlows -- Flexible waveform inversion software, Computers & Geosciences, Volume 115, 2018, Pages 88-95.

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