PaN, PaNOSC and ExPaNDS

Sharing knowledge with the open PaN e-learning platform

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These projects have received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823852 and No. 857641

Content

- Objectives
- On-going training activities: FAIR workshop
- PaN training portal concept
- Description of the e-learning platform: history, scope, examples, progress
- Added-value of the future PaN training portal

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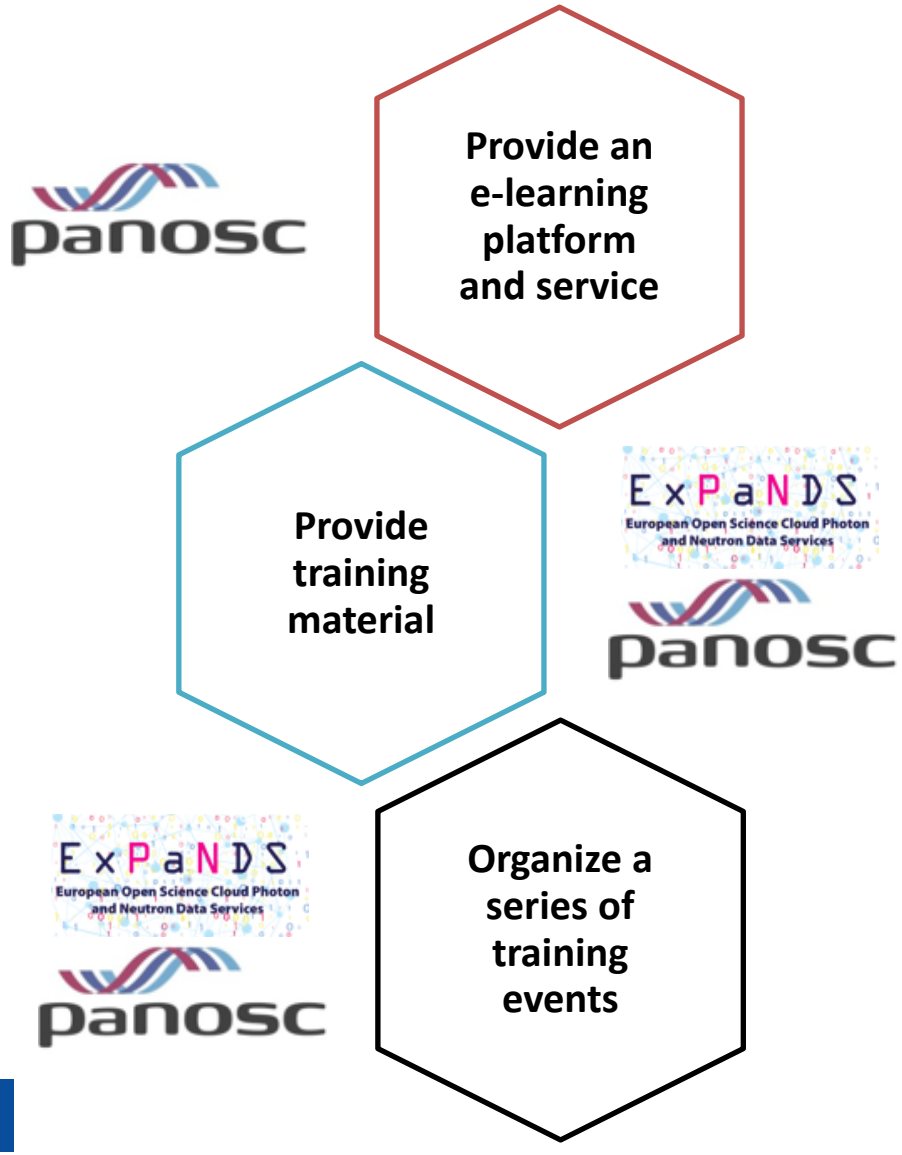
PaNOSC and ExPaNDS Training activities objectives



- **Provide an e-learning platform and service** to provide training to staff and users
- **Provide training material**
  - ✓ accessible to staff and users from national RIs
  - ✓ using EOSC data websites and e-learning platforms
  - ✓ to use the e-learning platform
  - ✓ to develop courses, and train staff at relevant RIs at specific workshops
  - ✓ to promote the FAIR principles and best practices
  - ✓ to promote services and capabilities of PaN facilities
- **Organize a series of training events** in :
  - ✓ data FAIR principles
  - ✓ data stewardship
  - ✓ data management
  - ✓ data analysis services integrated into the EOSC services
  - ✓ staff training on e-learning platform

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First training event: FAIR workshop (01-02/10/2020)

https://expands.eu/2020/09/09/expands-fair-workshops-1st-2nd-october-2020/

- **Target audience:** Instrument scientists and other facility staff
- **Overview of FAIR – key questions related to the data facilities produce** – What is FAIR? What's the difference between FAIR and Open? What are the benefits of FAIR for the PaN community? How do I start to make data FAIR? Examples connect the concept of FAIR to practice, highlighting the vital role facilities play in supporting FAIR for PaN research.
- **Exploration of the FAIR experiment** – What are the implications of FAIR for data management before, during, and after the experiment? When, where and how during the lifecycle of an experiment do we collect the metadata we need to document data and make them FAIR? What is active data management planning? How does it benefit both facilities and users and how does it help to make data FAIR?

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Ten simple rules for making training materials FAIR

Garcia et al. (2020) Ten simple rules for making training materials FAIR. **PLoS Comput Biol** 16(5): e1007854. https://doi.org/10.1371/journal.pcbi.1007854

- Guidelines **which apply the FAIR principles** to limitation experienced by trainers looking to find, (re)use and adapt learning materials.
- Guidelines **pertinent across domain** and include amongst others:
  - Plan to share your training materials online
  - Give your training materials a unique identity
  - Make your training materials contribution friendly
  - Improve findability of your training materials by properly describing them

Wiegers, Luc and van Gelder, Celia W. G. Illustration for the paper "Ten simple rules for making training materials FAIR". DOI 10.5281/zenodo.3593257

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Characteristics of the future PaN training portal

- The future PaN training portal:
  - **will be a registry that helps European PaN RIs** to promote their latest events and contribute to their catalogue of training material.
  - **will be an aggregator of training resources** (material and events)
  - **will include the e-learning platform** currently developed by PaNOSC to create and locally store training material
  - **will not be a repository and will not store (major) content** (the e-learning platform will do it locally if necessary). it will describe the training material and index links to content provider's training material (training provider's website or repositories as Github, Zenodo, Open Aire, etc).
- Future work on **collecting the material and events**, and on **metadata** definition to index the training content

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Vision

PaN training portal

Training events

- **Catalogue of training events** of interest for the PaN community (Online and f2f events)
- Workshops, MOOCs, summer schools, users' meetings …

Training material

- **Catalogue of training materials** of interest for the PaN community
- External links to content provider's website or repositories as Github, Zenodo, Open Aire, etc

E-learning platform

- **Tool available to create and store training material**
  - Moodle
  - Simulation tools
  - MediaWiki

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Scope & history of the e-learning platform

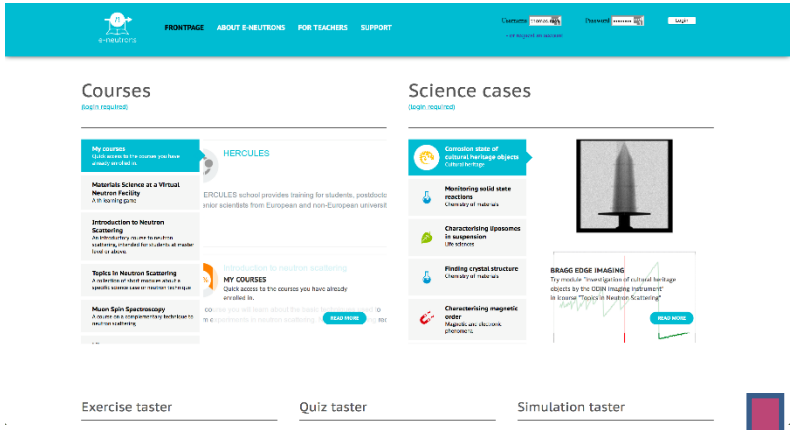
e-neutrons.org invented and developed primarily by *Linda Udby* (UCPH) & *Peter Willendrup* (DTU) in NMI3 and SINE2020

Introducing e-neutrons.org (2 min)

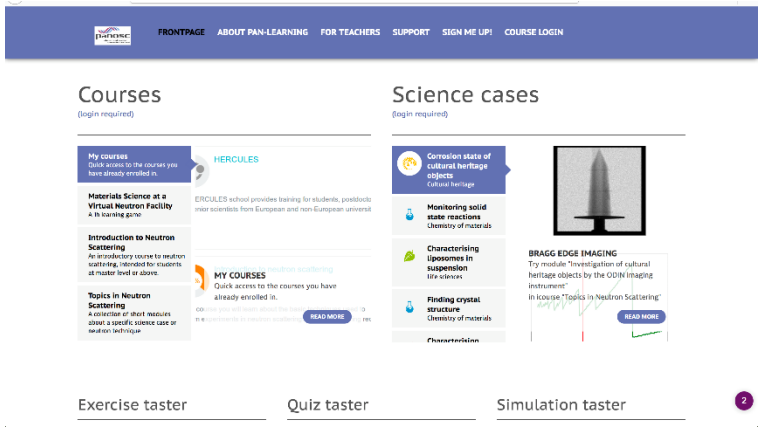
An introduction to the online learning platform.

https://www.youtube.com/watch?v=LvRVnPoAkNs&feature=youtu.be

https://e-neutrons.org



https://pan-learning.org



e-neutrons.org / pan-learning.org used used at multiple places, e.g.:

- University of Copenhagen
- Technical University of Delft
- Berlin school on neutron scattering
- SwednESS Summer schools.

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Components enable a rich e-learning environment

Components

MediaWiki

moodle

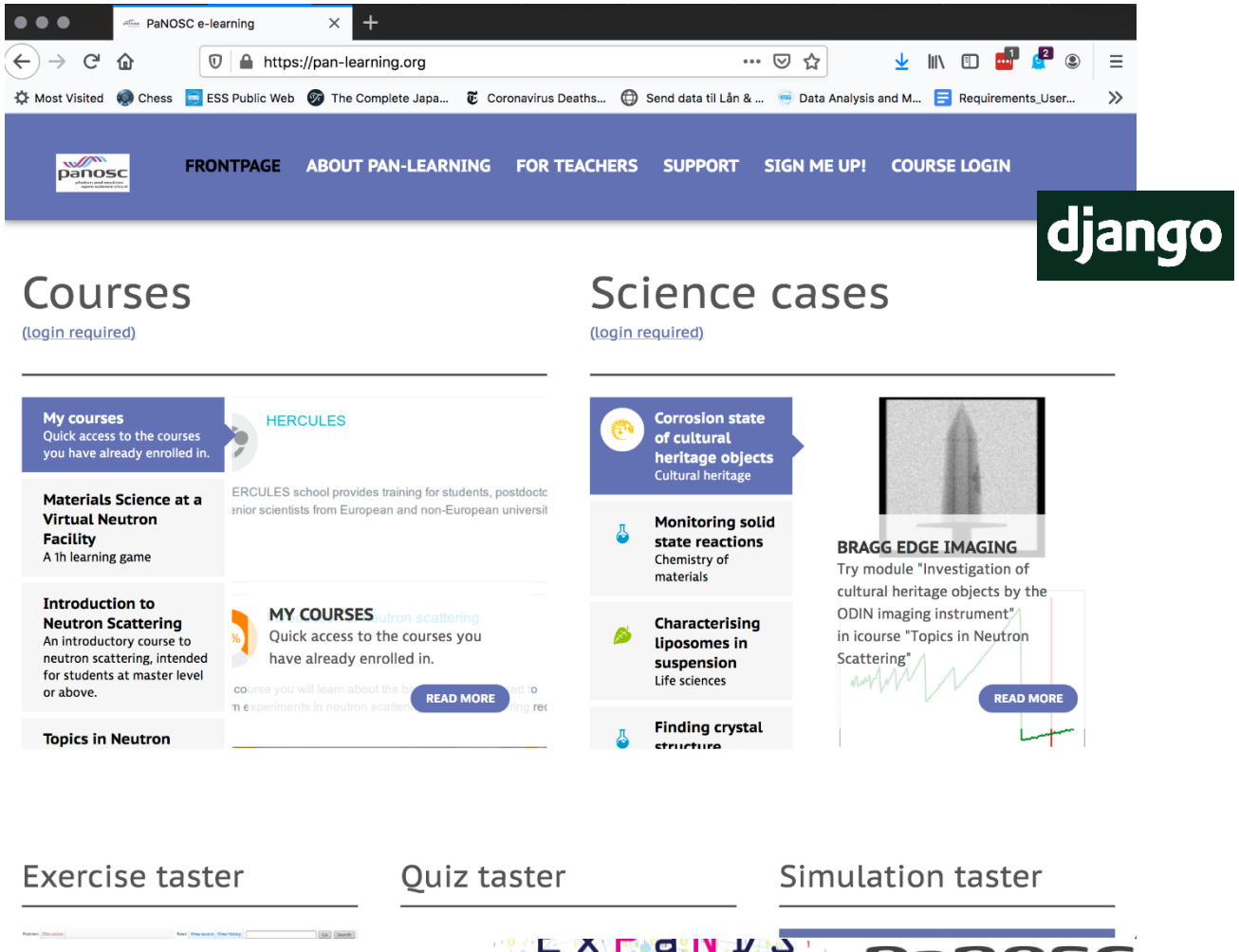
McStas

McXtrace

Work in progress:

jupyter

+ other simulation software



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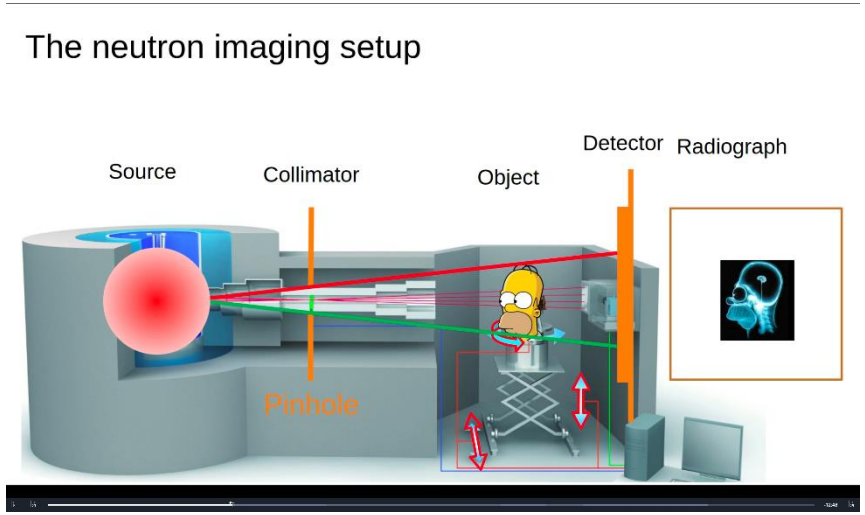
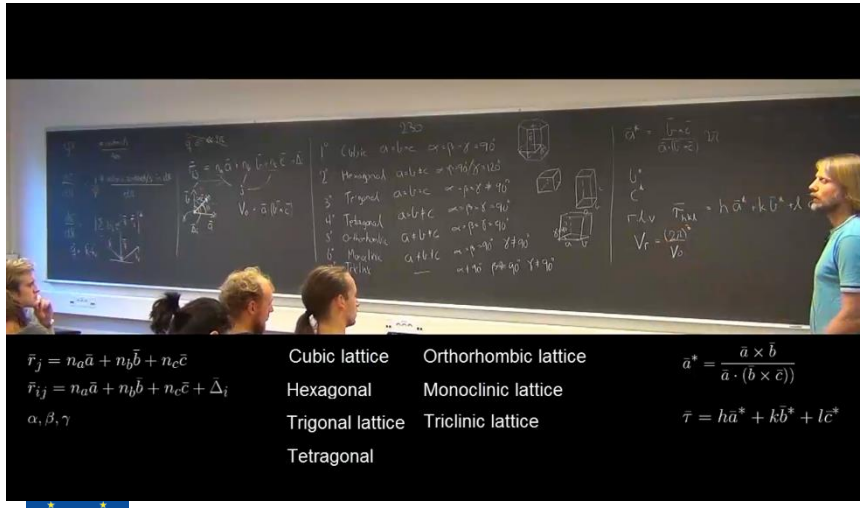
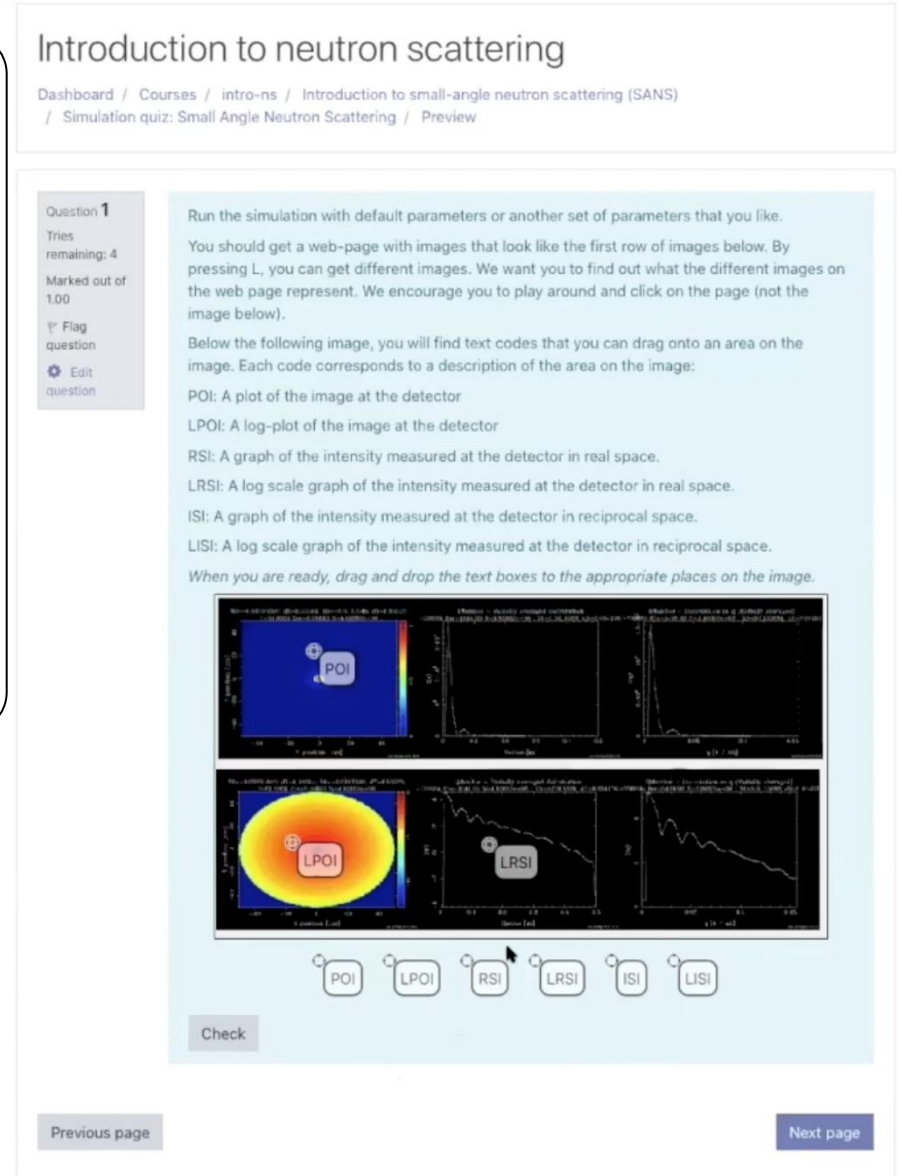




Types of learning materials

- ✓ Text book material
- ✓ Quizzes
- ✓ Slides
- ✓ Videos
- ✓ Annotated videos
- ✓ Virtual experiments
- ✓ Jupyter (scripting)



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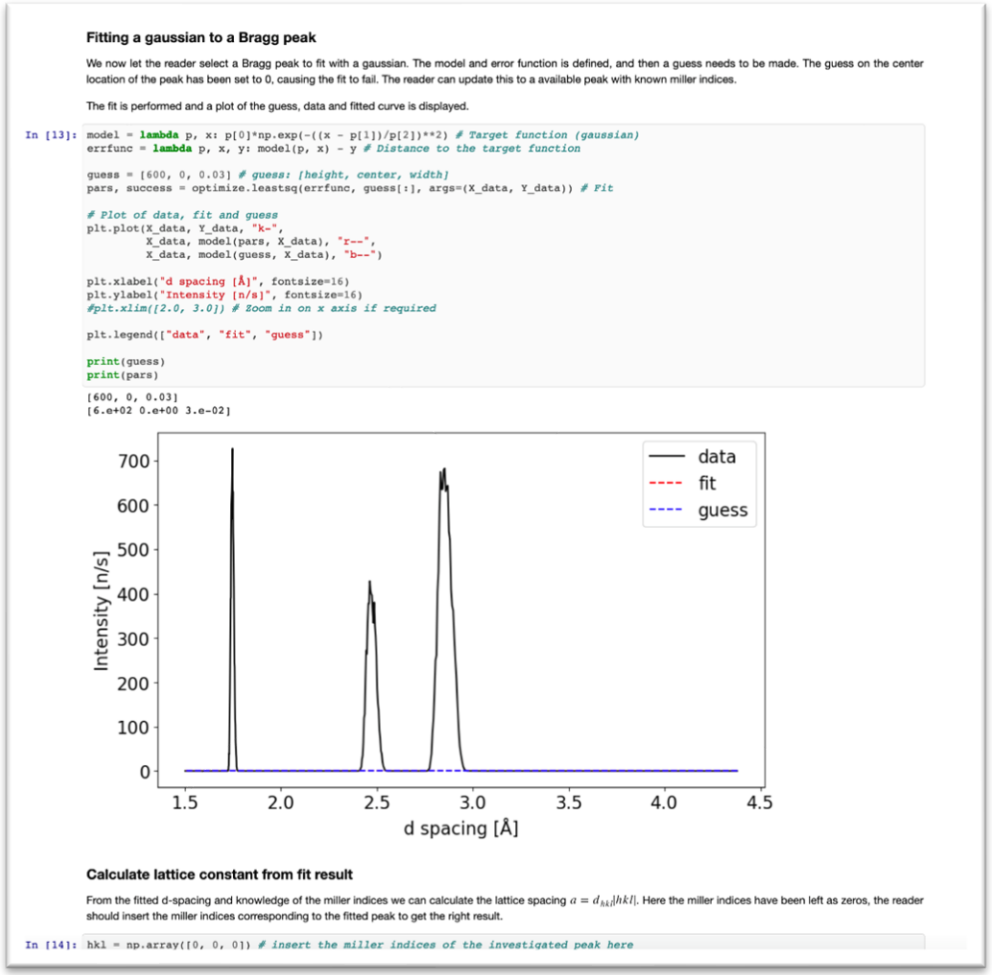
Progress

- e-neutrons.org migrated to ESS under the name of pan-learning.org
- devops and security improved
- Jupyter integrated
- Umbrella AAI integrated
- pan-learning.org -> EOSC service
- pan-learning.org workshop
- Separation of library of training material from e-learning platform
- New content



Fitting a gaussian to a Bragg peak

We now let the reader select a Bragg peak to fit with a gaussian. The model and error function is defined, and then a guess needs to be made. The guess on the center location of the peak has been set to 0, causing the fit to fail. The reader can update this to a available peak with known miller indices.

The fit is performed and a plot of the guess, data and fitted curve is displayed.

In [13]:
```
model = lambda p, x: p[0]*np.exp(-((x - p[1])/p[2])**2) # Target function (gaussian)
errfunc = lambda p, x, y: model(p, x) - y # Distance to the target function

guess = [600, 0, 0.03] # guess: [height, center, width]
pars, success = optimize.leastsq(errfunc, guess[:], args=(X_data, Y_data)) # Fit

# Plot of data, fit and guess
plt.plot(X_data, Y_data, "k-",
         X_data, model(pars, X_data), "r--",
         X_data, model(guess, X_data), "b--")

plt.xlabel("d spacing [Å]", fontsize=16)
plt.ylabel("Intensity [n/s]", fontsize=16)
#plt.xlim([2.0, 3.0]) # Zoom in on x axis if required

plt.legend(["data", "fit", "guess"])

print(guess)
print(pars)
```

```
[600, 0, 0.03]
[6.e+02 0.e+00 3.e-02]
```


Calculate lattice constant from fit result

From the fitted d-spacing and knowledge of the miller indices we can calculate the lattice spacing $a = d_{hkl}|hkl|$. Here the miller indices have been left as zeros, the reader should insert the miller indices corresponding to the fitted peak to get the right result.

In [14]:
```
hkl = np.array([0, 0, 0]) # insert the miller indices of the investigated peak here
```

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Added-value of the future PaN training portal

- **single entry point** to relevant training ressources and tools to create training material for the PaN community
- **centralised environment** for sharing training material and events information
- **effective gateway** to find relevant training events and ressources for the PaN community
- opportunity to **promote training events**
- contribute to a **growing catalogue** of PaN dedicated training materials

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Thank you!

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